I CLAIM:

1. A system of computing and rendering the nature of at least one specie selected from a group of diatomic molecules having at least one atom that is other than hydrogen, polyatomic molecules, molecular ions, polyatomic molecular ions, or molecular radicals, or any functional group therein, comprising physical, Maxwellian solutions of charge, mass, and current density functions of said specie, said system comprising:

processing means for processing physical, Maxwellian equations representing charge, mass, and current density functions of said specie; and

an output device in communication with the processing means for displaying said physical, Maxwellian solutions of charge, mass, and current density functions of said specie.

2. The system of claim 1 wherein the output device is a display that displays at least one of visual or graphical media.

3. The system of claim 2 wherein the display is at least one of static or dynamic.

4. The system of claim 3 wherein at least one of vibration and rotation is be displayed.

5. The system of claim 4 wherein displayed information is used to model reactivity and physical properties.

6. The system of claim 5, wherein the output device is a monitor, video projector, printer, or three-dimensional rendering device.

7. The system of claim 6 wherein displayed information is used to model other species and provides utility to anticipate their reactivity and physical properties.

8. The system of claim 7 wherein the processing means is a general purpose computer.

9. The system of claim 8 wherein the general purpose computer comprises a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or other storage device, an input means.

10. The system of claim 9, wherein the input means comprises a serial port, usb port, microphone input, camera input, keyboard or mouse.

11. The system of claim 10 wherein the processing means comprises a special purpose computer or other hardware system.

12. The system of claim 11 further comprising computer program products.

13. The system of claim 12 further comprising computer readable medium having embodied therein program code means.

14. The system of claim 13 wherein the computer readable media is any available media which can be accessed by a general purpose or special purpose computer.

15. The system of claim 14 wherein the computer readable media comprises at least one of RAM, ROM, EPROM, CD ROM, DVD or other optical disk storage, magnetic disk storage or other magnetic storage devices, or any other medium which can embody the desired program code means and which can be accessed by a general purpose or special purpose computer.

16. The system of claim 15 wherein the program code means comprises executable instructions and data which cause a general purpose computer or special purpose computer to perform a certain function of a group of functions.

17. The system of claim 16 wherein the program code is Mathematica programmed with an algorithm based on the physical solutions, and the computer is a PC.

18. The system of claim 17 wherein the algorithm is ParametricPlot3D[{2*Sqrt[1-z*z]*Cos[u],Sqrt[(1-z*z)]*Sin[u],z},{u,0,2* Pi},{z,-1,.9999}], and the rendering is viewed from different perspectives.

19. The system of claim 18 wherein the algorithms for viewing from different perspectives comprises Show[Out[1], ViewPoint->{x,y,z}] where x, y, and z are Cartesian coordinates.

20. The system of claim 19 wherein the physical, Maxwellian solutions of the charge, mass, and current density functions of said specie comprises a solution of the classical wave equation $\left[\nabla^2 - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right]\rho(r,\theta,\phi,t) = 0$ which is the equation of motion of the charge.

21. The system of claim 20 wherein the boundary constraint of the wave equation solution is nonradiation according to Maxwell's equations.

22. The system of claim 21 wherein the boundary condition is met for an ellipsoidal-time harmonic function when

$$\omega_n = \frac{\pi\hbar}{m_e A} = \frac{\hbar}{m_e ab}$$

where the area of an ellipse is

$$A = \pi ab$$

where $2b$ is the length of the semiminor axis and $2a$ is the length of the semimajor axis.

23. The system of claim 22 wherein the specie charge and current density functions, bond distance, and energies are solved from the Laplacian in ellipsoidal coordinates:

$$(\eta-\zeta)R_\xi\frac{\partial}{\partial\xi}(R_\xi\frac{\partial\phi}{\partial\xi}) + (\zeta-\xi)R_\eta\frac{\partial}{\partial\eta}(R_\eta\frac{\partial\phi}{\partial\eta}) + (\xi-\eta)R_\zeta\frac{\partial}{\partial\zeta}(R_\zeta\frac{\partial\phi}{\partial\zeta}) = 0\,.$$

with the constraint of nonradiation.

24. The system of claim 23 wherein each bond of the said specie defined as a molecular orbital (MO) has the ellipsoidal charge-density function given by

$$\sigma = \frac{q}{4\pi abc}\frac{1}{\sqrt{\frac{x^2}{a^4}+\frac{y^2}{b^4}+\frac{z^2}{c^4}}}$$

25. The system of claim 24 wherein the bonds of the said specie defined as a molecular orbital (MO) has the charge-density function comprising a linear combination of ellipsoids wherein the charge density of one said ellipsoid is given by

$$\sigma = \frac{q}{4\pi abc} \frac{1}{\sqrt{\frac{x^2}{a^4} + \frac{y^2}{b^4} + \frac{z^2}{c^4}}}$$

26. The system of claim 25 wherein the equation of motion has the parametric form

$$r(t) = \mathbf{i}a\cos\omega t + \mathbf{j}b\sin\omega t$$

27. The system of claim 26 wherein he force balance of the hydrogen-type molecular ion ellipsoidal MO is given by

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{pe^2}{8\pi\varepsilon_0} D$$

$$a = 2a_0$$

28. The system of claim 27 where the force constant k of a H_2^+-type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k = \frac{2e^2}{4\pi\varepsilon_o}$$

29. The system of claim 28 wherein the distance from the origin of the H_2-type-ellipsoidal-MO to each focus c' is given by :

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2a}} = \sqrt{\frac{aa_0}{2}}$$

30. The system of claim 29 wherein the internuclear distance $2c'$ is given by:

$$2c' = 2\sqrt{\frac{aa_0}{2}}$$

31. The system of claim 30 wherein the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ is given by:

$$b = \sqrt{a^2 - c'^2}$$

32. The system of claim 31 wherein the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ is given by:

$$e = \frac{c'}{a}$$

33. The system of claim 32 wherein the internuclear distance, $2c'$, which is the distance between the foci is

$$2c' = 2a_o;$$

the semiminor axis is

$$b = \sqrt{3}a_o, \text{ and}$$

the eccentricity, e, is

$$e = \frac{1}{2}.$$

34. The system of claim 33 wherein the potential energy of the electron in the central field of the protons at the foci is

$$V_e = \frac{-4e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}$$
$$= \frac{-4e^2}{8\pi\varepsilon_o c'}\ln\frac{a+c'}{a-c'} \quad ;$$
$$= \frac{-4e^2}{8\pi\varepsilon_o a_H}\ln 3 = -59.7575\ eV$$

The potential energy of the two protons is

$$V_p = \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} = \frac{e^2}{8\pi\varepsilon_o a_H} = 13.5984\ eV;$$

The kinetic energy of the electron is

$$T = \frac{2\hbar^2}{m_e a\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = \frac{2e^2}{8\pi\varepsilon_o a_H}\ln 3 = 29.8787\ eV, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_p$$

$$E_T = \frac{-e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[\left(4-\frac{4}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]$$
$$= \frac{-e^2}{8\pi e_o a_H}(4\ln 3-1-2\ln 3)$$
$$= -16.2803\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

35. The system of claim 34 wherein during bond formation, the electron undergoes a reentrant oscillatory orbit with vibration of the protons, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{\frac{e^2}{8\pi\varepsilon_o a_H}(4\ln 3-1-2\ln 3)\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{2e^2}{4\pi\varepsilon_o\left(2a_H\right)^3}}{m_e}}{m_e c^2}}\right]-\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$
$$= -16.2803\ eV - 0.118811\ eV + \frac{1}{2}(0.29282\ eV)$$
$$= -16.2527\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

36. The system of claim 35 wherein the bond dissociation energy, E_D, is the difference between the total energy of the hydrogen atom and E_T:

$$E_D = E(H) - E_T = 2.654\ eV$$

wherein the total energy of a hydrogen atom is $E(H) = -13.59844\ eV$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

37. The system of claim 36 wherein the H_2^+-type ellipsoidal MO and the hydrogen atomic orbital (AO) serve as basis functions for the MOs of specie.

38. The system of claim 37 wherein the MO must (1) be a solution of Laplace's equation to give a equipotential energy surface, (2) correspond to an orbital solution of the Newtonian equation of motion in an inverse-radius-squared central field having a constant total energy, (3) be stable to radiation, and (4) conserve the electron angular momentum of $\hbar$.

39. The system of claim 38 wherein the potential energy of electron in the central field of the protons at the foci is

$$V_e = \frac{-4e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = \frac{-4e^2}{8\pi\varepsilon_o c'}\ln\frac{a+c'}{a-c'};$$

The potential energy of the two protons is

$$V_p = \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} = \frac{e^2}{8\pi\varepsilon_0 c'};$$

The kinetic energy of the electron is

$$T = \frac{2\hbar^2}{m_e a\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = \frac{2\hbar^2}{m_e a c'}\ln\frac{a+c'}{a-c'}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_p$$

$$E_T = \frac{-e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[\left(4-\frac{4}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right] = \frac{-e^2}{8\pi\varepsilon_o c'}\left[\left(4-\frac{4}{a}\right)\ln\frac{a+c'}{a-c'}-1\right].$$

40. The system of claim 39 wherein during bond formation, the electron undergoes a reentrant oscillatory orbit with vibration of the protons, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{ \frac{-e^2}{8\pi\varepsilon_o c'}\left[\left(4-\frac{4}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{2e^2}{4\pi\varepsilon_o (a)^3}}{m_e}}{m_e c^2}}\right]-\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

41. The system of claim 40 wherein the force balance equation derived of a H_2-type ellipsoidal MO is given by

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{pe^2}{8\pi\varepsilon_o a b^2} D + \frac{\hbar^2}{2 m_e a^2 b^2} D$$

$$a = \frac{a_0}{p}$$

42. The system of claim 41 where the force constant k of a H_2-type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k = \frac{2e^2}{4\pi\varepsilon_o}$$

43. The system of claim 42 wherein the distance from the origin of the H_2-type-ellipsoidal-MO to each focus c' is given by :

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2a}} = \sqrt{\frac{a a_0}{2}}$$

44. The system of claim 43 wherein the internuclear distance $2c'$ is given by:

$$2c' = 2\sqrt{\frac{a a_0}{2}}$$

45. The system of claim 44 wherein the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ is given by:

$$b = \sqrt{a^2 - c'^2}$$

46. The system of claim 45 wherein the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ is given by:

$$e = \frac{c'}{a}$$

47. The system of claim 46 wherein the internuclear distance, $2c'$, which is the distance between the foci is

$$2c' = \sqrt{2}a_o;$$

the semiminor axis is

$b = \frac{1}{\sqrt{2}} a_o$, and

the eccentricity, e, is

$$e = \frac{1}{\sqrt{2}}.$$

48. The system of claim 47 wherein the potential energy of the two electrons in the central field of the protons at the foci is

$$V_e = \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = -67.8358\ eV;$$

The potential energy of the two protons is

$$V_p = \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} = 19.2415\ eV;$$

The kinetic energy of the electrons is

$T = \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = 33.9179\ eV$, and

The energy, V_m, of the magnetic force between the electrons is

$$V_m = \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = -16.9589\ eV, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -13.60\ eV\left[\left(2p^2\sqrt{2} - p^2\sqrt{2} + \frac{p^2\sqrt{2}}{2}\right)\ln\frac{\sqrt{2}+1}{\sqrt{2}-1} - p^2\sqrt{2}\right] = -p^2 31.63$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

49. The system of claim 48 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the protons, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{\frac{e^2}{8\pi\varepsilon_o a_0}\left[\left(2\sqrt{2} - \sqrt{2} + \frac{\sqrt{2}}{2}\right)\ln\frac{\sqrt{2}+1}{\sqrt{2}-1} - \sqrt{2}\right]\left[1 + \sqrt{\frac{2\hbar\sqrt{\frac{e^2}{4\pi\varepsilon_o a_0^3}}}{m_e c^2}}\right] - \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

$$= -31.635\ eV - 0.326469\ eV + \frac{1}{2}(0.56764\ eV)$$

$$= -31.6776\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

50. The system of claim 49 wherein the bond dissociation energy, E_D, is the difference between the total energy of the hydrogen atoms and E_T:

$$E_D = E(2H[a_H]) - E_T = 4.478\ eV$$

wherein the total energy of two hydrogen atoms is $E(2H[a_H]) = -27.21\ eV$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

51. The system of claim 50 wherein the H_2-type ellipsoidal MO and the hydrogen atomic orbital (AO) serve as basis functions for the MOs of the specie.

52. The system of claim 51 wherein the MO must (1) be a solution of Laplace's equation to give a equipotential energy surface, (2) correspond to an orbital solution of the Newtonian equation of motion in an inverse-radius-squared central field having a constant total energy, (3) be stable to radiation, and (4) conserve the electron angular momentum of $\hbar$.

53. The system of claim 52 wherein the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e = \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}};$$

The potential energy of the two nuclei is

$$V_p = \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}};$$

The kinetic energy of the electrons is

$$T = \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -\frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right] = -\frac{e^2}{8\pi\varepsilon_0 c'}\left[\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right].$$

54. The system of claim 53 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{ \frac{e^2}{8\pi\varepsilon_0 c'}\left[\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{e^2}{4\pi\varepsilon_o a^3}}}{m_e c^2}}\right]-\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

55. The system of claim 54 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{\overline{E}}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{ \frac{e^2}{8\pi\varepsilon_0 c'}\left[\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{e^2}{4\pi\varepsilon_o b^3}}}{m_e c^2}}\right]-\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

56. The system of claim 55 wherein the energy of the MO is matched to that of the outermost atomic orbital of a bonding heteroatom in the case where a minimum energy is achieved with a direct bond to the AO.

57. The system of claim 56 wherein the MO is continuous with the AO containing paired electrons that do not participate in the bond, and said paired electrons provide a means for the energy matched MO to form a continuous equipotential energy surface.

58. The system of claim 57 wherein an independent MO is formed such that the AO force balance causes the remaining electrons to be at lower energy and a smaller radius.

59. The system of claim 58 wherein at least two atomic orbital hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum.

60. The system of claim 59 wherein at least two atomic orbital hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum.

61. The system of claim 60 wherein at least two atomic orbitals hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum, and the sharing of electrons between two or more such orbitals to form a MO permits the participating hybridized orbitals to decrease in energy through a decrease in the radius of one or more of the participating orbitals.

62. The system of claim 61 where the force constant k' of a H_2-type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{c_1 c_2 2e^2}{4\pi\varepsilon_o}$$

where c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of the chemical bond.

63. The system of claim 62 where the distance from the origin of the MO to each focus c' is given by:

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2k' a}} = \sqrt{\frac{aa_0}{2k'}};$$

the internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2k'}};$$

the length of the semiminor axis of the prolate spheroidal MO $b = c$ is given by

$b = \sqrt{a^2 - c'^2}$, and

and, the eccentricity, e, is

$$e = \frac{c'}{a}.$$

64. The system of claim 63 wherein the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}};$$

The potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}};$$

The kinetic energy of the electrons is

$$T = n_1 c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]$$
$$= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

65. The system of claim 64 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{c_1 c_2 e^2}{4\pi\varepsilon_o a^3}}{m_e}}{m_e c^2}}\right]-n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

66. The system of claim 65 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{c_1 c_2 e^2}{4\pi\varepsilon_o b^3}}{m_e}}{m_e c^2}}\right]-n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

67. The system of claim 66 wherein a hybridized shell comprises a linear combination of the electrons of at least two atomic-orbital shells.

68. The system of claim 67 wherein the radius of the hybridized shell is calculated from the Coulombic energy equation by considering that the central field decreases by an integer for

each successive electron of the shell and the total energy of the shell is equal to the total Coulombic energy of the initial AO electrons.

69. The system of claim 68 wherein the total energy $E_T\left(atom, msp^3\right)$ (m is the integer of the valence shell) of the AO electrons and the hybridized shell is given by the sum of energies of successive ions of the atom over the n electrons comprising total electrons of the at least two AO shells

70. The system of claim 69 wherein the radius r_{msp^3} of the hybridized shell is given by:

$$r_{msp^3} = \sum_{q=Z-n}^{Z-1} \frac{(Z-q)e^2}{8\pi\varepsilon_0 E_T\left(atom, msp^3\right)}$$

71. The system of claim 70 wherein the Coulombic energy $E_{Coulomb}\left(atom, msp^3\right)$ of the outer electron of the $atom\ msp^3$ shell is given by

$$E_{Coulomb}\left(atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}}$$

72. The system of claim 71 wherein the during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO) and the energy change the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r_n of the AO electron:

$$E(magnetic) = \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_n\right)^3} = \frac{8\pi\mu_o\mu_B^2}{\left(r_n\right)^3}$$

73. The system of claim 72 wherein the energy $E\left(atom, msp^3\right)$ of the outer electron of the $atom\ msp^3$ shell is given by the sum of $E_{Coulomb}\left(atom, msp^3\right)$ and $E(magnetic)$:

$$E\left(atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_n\right)^3}$$

74. The system of claim 73 wherein at least two atomic orbitals hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum, and the sharing of electrons between two or more such hybridized orbitals to form a MO permits the participating hybridized orbitals to decrease in energy through a decrease in the radius of one or more of the participating orbitals; the total energy of the hybridized orbitals is given by the sum of $E\left(atom, msp^3\right)$ and the next energies of successive ions of the atom over the n electrons comprising total electrons of the at least two initial AO shells; is the sum of the first energy of the atom and the hybridization energy.

75. The system of claim 74 wherein the sharing of electrons between two *atom* msp^3 HOs to form an atom-atom-bond MO permits each participating hybridized orbital to decrease in radius and energy.

76. The system of claim 75 wherein in order to further satisfy the potential, kinetic, and orbital energy relationships, each *atom* msp^3 HO donates an excess of 25% per bond of its electron density to the atom-atom-bond MO to form an energy minimum wherein the atom-atom bond comprises one of a single, double, or triple bond.

77. The system of claim 76 wherein the radius of the hybridized shell is calculated from the Coulombic energy equation by considering that the central field decreases by an integer for each successive electron of the shell and the total energy of the shell is equal to the total Coulombic energy of the initial AO electrons and the hybridization energy.

78. The system of claim 77 wherein the total energy $E_T\left(mol.atom, msp^3\right)$ (m is the integer of the valence shell) of the HO electrons is given by the sum of energies of successive ions of the atom over the n electrons comprising total electrons of the at least two initial AO shells and the hybridization energy.

79. The system of claim 78 wherein the radius r_{msp^3} of the hybridized shell is given by:

$$r_{msp^3} = \left(\sum_{q=Z-n}^{Z-1} (Z-q) - s(0.25) \right) \frac{e^2}{8\pi\varepsilon_0 E_T\left(mol.atom, msp^3\right)}$$

where $s = 1,2,3$ for a single, double, and triple bond, respectively.

80. The system of claim 79 wherein the Coulombic energy $E_{Coulomb}\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by

$$E_{Coulomb}\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}}$$

81. The system of claim 80 wherein the during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO) and the energy change the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r_n of the AO electron:

$$E(magnetic) = \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_n\right)^3} = \frac{8\pi\mu_o\mu_B^2}{\left(r_n\right)^3}$$

82. The system of claim 81 wherein the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$:

$$E\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_n\right)^3}$$

83. The system of claim 82 wherein $E_T\left(atom - atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of the atom-atom-bond MO is given by the difference between $E\left(mol.atom, msp^3\right)$ and $E\left(atom, msp^3\right)$.

$$E_T\left(atom - atom, msp^3\right) = E\left(mol.atom, msp^3\right) - E\left(atom, msp^3\right)$$

84. The system of claim 83 wherein to meet an energy matching condition for all MOs at all HOs, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell of each bonding atom must be the average of $E\left(mol.atom, msp^3\right)$ for two different values of s:

$$E\left(mol., msp^3\right) = \frac{E\left(mol(s_1), msp^3\right) + E\left(mol(s_2), msp^3\right)}{2} \qquad (14.512)$$

85. The system of claim 84 wherein $E_T\left(atom-atom,msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of each atom-atom-bond MO, is average of $E_T\left(atom-atom,msp^3\right)$ for two different values of s:

$$E_T\left(atom-atom,msp^3\right)=\frac{E_T\left(atom-atom(s_1),msp^3\right)+E_T\left(atom-atom(s_2),msp^3\right)}{2}$$

86. The system of claim 85 wherein the radius r_{msp^3} of the *atom* msp^3 shell of each bonding atom is given by the Coulombic energy using the initial energy $E_{Coulomb}\left(atom,msp^3\right)$ and $E_T\left(atom-atom,msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of each atom-atom-bond MO:

$$r_{msp^3}=\frac{-e^2}{8\pi\varepsilon_0 a_0\left(E_{Coulonb}\left(atom,msp^3\right)+E_T\left(atom-atom,msp^3\right)\right)} \tag{14.514}$$

87. The system of claim 86 wherein the Coulombic energy $E_{Coulomb}\left(mol.atom,msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by

$$E_{Coulomb}\left(mol.atom,msp^3\right)=\frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}}$$

88. The system of claim 87 wherein the during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO) and the energy change the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r_n of the AO electron:

$$E(magnetic)=\frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_n\right)^3}=\frac{8\pi\mu_o\mu_B^2}{\left(r_n\right)^3}.$$

89. The system of claim 88 wherein the energy $E\left(mol.atom,msp^3\right)$ of the outer electron of

the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$:

$$E\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_n\right)^3}$$

90. The system of claim 89 wherein $E_T\left(atom-atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of the atom-atom-bond MO is given by the difference between $E\left(mol.atom, msp^3\right)$ and $E\left(atom, msp^3\right)$.

$$E_T\left(atom-atom, msp^3\right) = E\left(mol.atom, msp^3\right) - E\left(atom, msp^3\right)$$

91. The system of claim 90 wherein $E_{Coulomb}\left(mol.atom, msp^3\right)$ is one of is one of $E_{Coulomb}\left(C_{ethylene}, 2sp^3\right)$, $E_{Coulomb}\left(C_{ethane}, 2sp^3\right)$, $E_{Coulomb}\left(C_{acetylene}, 2sp^3\right)$, and $E_{Coulomb}\left(C_{alkane}, 2sp^3\right)$;

$E_{Coulomb}\left(atom, msp^3\right)$ is one of $E_{Coulomb}\left(C, 2sp^3\right)$ and $E_{Coulomb}\left(Cl, 3sp^3\right)$;

$E\left(mol.atom, msp^3\right)$ is one of $E\left(C_{ethylene}, 2sp^3\right)$, $E\left(C_{ethane}, 2sp^3\right)$, $E\left(C_{acetylene}, 2sp^3\right)$ $E\left(C_{alkane}, 2sp^3\right)$;

$E\left(atom, msp^3\right)$ is one of and $E\left(C, 2sp^3\right)$ and $E\left(Cl, 3sp^3\right)$;

$E_T\left(atom-atom, msp^3\right)$ is one of $E\left(C-C, 2sp^3\right)$, $E\left(C=C, 2sp^3\right)$, and. $E\left(C\equiv C, 2sp^3\right)$;

atom msp^3 is one of $C2sp^3$, $Cl3sp^3$

$E_T\left(atom-atom(s_1), msp^3\right)$ is $E_T\left(C-C, 2sp^3\right)$ and $E_T\left(atom-atom(s_2), msp^3\right)$ is $E_T\left(C=C, 2sp^3\right)$, and

r_{msp^3} is one of r_{C2sp^3}, $r_{ethane2sp^3}$, $r_{ethylene2sp^3}$, $r_{acetylene2sp^3}$, $r_{alkane2sp^3}$, and r_{Cl3sp^3},

92. The system of claim 91 wherein the energy of the MO is matched to that of the outermost atomic orbital or hybridized orbital of a bonding atom in the case where a minimum energy is achieved with a direct bond to the AO or HO.

93. The system of claim 92 wherein the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o \sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}};$$

The potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\varepsilon_o \sqrt{a^2-b^2}};$$

The kinetic energy of the electrons is

$$T = n_1 c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms plus $E(AO)$:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -\frac{n_1 e^2}{8\pi\varepsilon_o \sqrt{a^2-b^2}} \left[c_1 c_2 \left(2 - \frac{a_0}{a}\right) \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} - 1 \right] + E(AO)$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'} \left[c_1 c_2 \left(2 - \frac{a_0}{a}\right) \ln \frac{a+c'}{a-c'} - 1 \right] + E(AO)$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital to which the MO is energy matched.

94. The system of claim 93 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib}, \text{ and}$$

the total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc} + E(AO).$$

95. The system of claim 94 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

the total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2 - \frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'} - 1\right]\left[1 + \sqrt{\frac{2\hbar\sqrt{\frac{c_1 c_2 e^2}{4\pi\varepsilon_o a^3}}{m_e}}{m_e c^2}}\right] - n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\} + E(AO)$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital to which the MO is energy matched.

96. The system of claim 95 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

the total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{ \frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2 \left(2 - \frac{a_0}{a}\right) \ln\frac{a+c'}{a-c'} - 1 \right]\left[1 + \sqrt{\frac{2\hbar\sqrt{\frac{c_1 c_2 e^2}{4\pi\varepsilon_o b^3}}\, m_e}{m_e c^2}} \right] - n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}} \right\} + E(AO)$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital or hybridized atomic orbital or said orbital or hybridized orbital and the energy change with the formation of the bond by one or more of the orbital electrons to match the energies of the said orbital and the MO.

97. The system of claim 96 wherein $E(AO)$, the energy of the at least one atomic orbital or hybridized atomic orbital or said orbital or hybridized orbital and the energy change with the formation of the bond by one or more of the orbital electrons to match the energies of the said orbital and the MO, is at least one from the group of

$E(AO) = E(O2p\ shell) = -E(ionization;\ O) = -13.6181\ eV$;

$E(AO) = E(N2p\ shell) = -E(ionization;\ N) = -14.53414\ eV$;

$E(AO) = E(C, 2sp^3) = -14.63489\ eV$;

$E_T(AO) = E_{Coulomb}(Cl, 3sp^3) = -14.60295\ eV$;

$E_T(AO) = E(ionization;\ C) + E(ionization;\ C^+)$;

$E_T(AO) = E(C_{ethane}, 2sp^3) = -15.35946\ eV$;

$E_T(AO) = +E(C_{ethylene}, 2sp^3) - E(C_{ethylene}, 2sp^3)$;

$E_T(AO) = E(C, 2sp^3) - 2E_T(C = C, 2sp^3) = -14.63489\ eV - (-2.26758\ eV)$;

$E_T(AO) = E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) = 16.20002\ eV$;

$E_T(AO) = E(C, 2sp^3) - 2E_T(C \equiv C, 2sp^3) = -14.63489\ eV - (-3.13026\ eV)$;

$E_T(AO) = E(C_{benzene}, 2sp^3) - E(C_{benzene}, 2sp^3)$;

$E_T(AO) = E(C, 2sp^3) - E_T(C = C, 2sp^3) = -14.63489\ eV - (-1.13379\ eV)$, and $E_T(AO) = E(C_{alkane}, 2sp^3) = -15.56407\ eV$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

98. The system of claim 97 wherein $c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2k' a}} = \sqrt{\frac{aa_0}{2k'}}$ is substituted into E_T to give

$$E_T = -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} - 1\right] + E(AO)$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'} - 1\right] + E(AO)$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0\sqrt{\frac{aa_0}{2k'}}}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2k'}}}{a-\sqrt{\frac{aa_0}{2k'}}} - 1\right] + E(AO)$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital or hybridized atomic orbital to which the MO is energy matched.

99. The system of claim 98 wherein $E(basis\ energies)$ is given by the sum of a first integer q_1 times the total energy of H_2 and a second integer q_2 times the total energy of H, minus a third integer q_3 times the total energy of $E(AO)$ where the first integer can be 1,2,3..., and each of the second and third integers can be 0,1,2,3....

100. The system of claim 99 wherein E_T is set equal to $E(basis\ energies)$, and the semimajor axis a is solved.

101. The system of claim 100 wherein the semimajor axis a is solved from the equation of the form:

$$E_T = -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]+E(AO)$$

$$=-\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]+E(AO)$$

$$=-\frac{n_1 e^2}{8\pi\varepsilon_0\sqrt{\frac{aa_0}{2k'}}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2k'}}}{a-\sqrt{\frac{aa_0}{2k'}}}-1\right]+E(AO)=E(\textit{basis energies})$$

102. The system of claims 101 and 63 wherein the distance from the origin of the H_2-type-ellipsoidal-MO to each focus c', the internuclear distance $2c'$, and the length of the semiminor axis of the prolate spheroidal H_2-type MO $b=c$ are solved from the semimajor axis a.

103. The system of claims 102 where the number of equivalent bonds of the MO n_1 each comprising an H_2-type ellipsoidal MO is an integer greater than one.

104. The system of claims 103 where the fraction c_1 of a H_2-type ellipsoidal MO is 1. 0.75, 0.5, and 0.75/2.

105. The system of claims 104 where the factor c_2 of a H_2-type ellipsoidal MO is given by one of the list of 1 and the ratio of the ionization energy of at least one atom of the bond and 13.605804 eV, the Coulombic energy between the electron and proton of H to meet the equipotential condition of the union of the H_2-type-ellipsoidal-MO and the AO of the atom, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

106. The system of claim 105 where the factor c_2 of a H_2-type ellipsoidal MO is 0.936127, the ratio of the ionization energy of N 14.53414 eV and 13.605804 eV, the Coulombic energy between the electron and proton of H;

0.91771, the ratio of 14.82575 eV, $E_{Coulomb}\left(C,2sp^3\right)$ and 13.605804 eV, the Coulombic energy between the electron and proton of H;

0.93172, the ratio of 14.60295 eV, $E_{Coulomb}\left(Cl,3sp^3\right)$ given by Eq. (13.759), and 13.605804 eV, the Coulombic energy between the electron and proton of H;

0.87495, the ratio of 15.55033 eV, $E_{Coulomb}\left(C_{ethane},2sp^3\right)$ and 13.605804 eV, the Coulombic energy between the electron and proton of H;

0.85252, the ratio of 15.95955 eV, $E_{Coulomb}\left(C_{ethylene},2sp^3\right)$ and 13.605804 eV, the Coulombic energy between the electron and proton of H;

0.85252, the ratio of 15.95955 eV, $E_{Coulomb}\left(C_{benzene},2sp^3\right)$ and 13.605804 eV, the Coulombic energy between the electron and proton of H, or

0.86359, the ratio of 15.55033 eV, $E_{Coulomb}\left(C_{alkane},2sp^3\right)$ and 13.605804 eV, the Coulombic energy between the electron and proton of H, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

107. The system of claim 106 where the fraction c_1 of a H_2-type ellipsoidal MO is such that the orbital energy E for each elliptical cross section of the prolate spheroidal MO is given by the sum of the kinetic T and potential V energies; $E=T+V$ is constant; the orbit is closed such that $T<|V|$; the time average of the kinetic energy, $<T>$, for elliptic motion in an inverse-squared field is $1/2$ that of the time average of the magnitude of the potential energy, $|<V>|$ ($<T>=1/2|<V>|$), and in the case that the energy of the MO is matched to at least one atomic orbital (AO), $E=T+V$, and for all points on the AO, $|E|=T=1/2|V|$.

108. The system of claim 107 where the energy of the MO is matched to at least one atomic orbital (AO) such that $E=T+V$, and for all points on the AO, $|E|=T=1/2|V|$.

109. A system of claim 108 of computing and rendering the nature of bound atomic and atomic ionic electrons from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration, comprising:

processing means for processing and solving the equations for charge, mass, and current density functions of electron(s) in a selected atom or ion, wherein the equations are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration; and

a display in communication with the processing means for displaying the current and charge density representation of the electron(s) of the selected atom or ion.

110. The system of claim 109 wherein the physical, Maxwellian solutions of the charge, mass, and current density functions of atoms and atomic ions comprises a solution of the classical wave equation $\left[\nabla^2 - \frac{1}{v^2}\frac{\delta^2}{\delta t^2}\right]\rho(r,\theta,\phi,t) = 0$ which is the equation of motion of the charge.

111. The system of claim 110, wherein the time, radial, and angular solutions of the wave equation are separable.

112. The system of claim 111, wherein the boundary constraint of the wave equation solution is nonradiation according to Maxwell's equations.

113. The system of claim 112, wherein a radial function that satisfies the boundary condition is a radial delta function

$$f(r) = \frac{1}{r^2}\delta(r - r_n).$$

114. The system of claim 113, wherein the boundary condition is met for a time harmonic function when the relationship between an allowed radius and the electron wavelength is given by

$$2\pi r_n = \lambda_n,$$

$$\omega = \frac{\hbar}{m_e r^2}, \text{ and}$$

$$v = \frac{\hbar}{m_e r}$$

where ω is the angular velocity of each point on the electron surface, v is the velocity of each point on the electron surface, and r is the radius of the electron.

115. The system of claim 114, wherein the spin function is given by the uniform function $Y_0^0(\phi,\theta)$ comprising angular momentum components of $\mathbf{L}_{xy}=\frac{\hbar}{4}$ and $\mathbf{L}_z=\frac{\hbar}{2}$.

116. The system of claim 115, wherein the atomic and atomic ionic charge and current density functions of bound electrons are described by a charge-density (mass-density) function which is the product of a radial delta function, two angular functions (spherical harmonic functions), and a time harmonic function:

$$\rho(r,\theta,\phi,t)=f(r)A(\theta,\phi,t)=\frac{1}{r^2}\delta(r-r_n)A(\theta,\phi,t); \qquad A(\theta,\phi,t)=Y(\theta,\phi)k(t)$$

wherein the spherical harmonic functions correspond to a traveling charge density wave confined to the spherical shell which gives rise to the phenomenon of orbital angular momentum.

117. The system of claim 116, wherein based on the radial solution, the angular charge and current-density functions of the electron, $A(\theta,\phi,t)$, must be a solution of the wave equation in two dimensions (plus time),

$$\left[\nabla^2-\frac{1}{v^2}\frac{\delta^2}{\delta t^2}\right]A(\theta,\phi,t)=0$$

where $\rho(r,\theta,\phi,t)=f(r)A(\theta,\phi,t)=\frac{1}{r^2}\delta(r-r_n)A(\theta,\phi,t)$ and $A(\theta,\phi,t)=Y(\theta,\phi)k(t)$

$$\left[\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)_{r,\phi}+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)_{r,\theta}-\frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right]A(\theta,\phi,t)=0$$

where v is the linear velocity of the electron.

118. The system of claim 117, wherein the charge-density functions including the time-function factor are

$\ell=0$

$$\rho(r,\theta,\phi,t)=\frac{e}{8\pi r^2}[\delta(r-r_n)]\left[Y_0^0(\theta,\phi)+Y_\ell^m(\theta,\phi)\right]$$

$\ell \neq 0$

$$\rho(r,\theta,\phi,t)=\frac{e}{4\pi r^2}[\delta(r-r_n)]\left[Y_0^0(\theta,\phi)+\mathrm{Re}\left\{Y_\ell^m(\theta,\phi)e^{i\omega_n t}\right\}\right]$$

where $Y_\ell^m(\theta,\phi)$ are the spherical harmonic functions that spin about the z-axis with angular frequency ω_n with $Y_0^0(\theta,\phi)$ the constant function

$\mathrm{Re}\left\{Y_\ell^m(\theta,\phi)e^{i\omega_n t}\right\}=P_\ell^m(\cos\theta)\cos\left(m\phi+\omega_n' t\right)$ where to keep the form of the spherical harmonic as a traveling wave about the z-axis, $\omega_n'=m\omega_n$.

119. The system of claim 118, wherein the spin and angular moment of inertia, I, angular momentum, L, and energy, E, for quantum number ℓ are given by

$\ell = 0$

$$I_z = I_{spin} = \frac{m_e r_n^{\,2}}{2}$$

$$L_z = I\omega \mathbf{i}_z = \pm\frac{\hbar}{2}$$

$$E_{rotational} = E_{rotational,\,spin} = \frac{1}{2}\left[I_{spin}\left(\frac{\hbar}{m_e r_n^{\,2}}\right)^2\right] = \frac{1}{2}\left[\frac{m_e r_n^{\,2}}{2}\left(\frac{\hbar}{m_e r_n^{\,2}}\right)^2\right] = \frac{1}{4}\left[\frac{\hbar^2}{2I_{spin}}\right]$$

$\ell \neq 0$

$$I_{orbital} = m_e r_n^{\,2}\left[\frac{\ell(\ell+1)}{\ell^2+\ell+1}\right]^{\frac{1}{2}}$$

$$L_z = m\hbar$$

$$L_{z\ total} = L_{z\ spin} + L_{z\ orbital}$$

$$E_{rotational,\,orbital} = \frac{\hbar^2}{2I}\left[\frac{\ell(\ell+1)}{\ell^2+2\ell+1}\right]$$

$$T = \frac{\hbar^2}{2m_e r_n^2}$$

$$\left\langle E_{rotational,\,orbital}\right\rangle = 0\,.$$

120. The system of claim 119, wherein the force balance equation for one-electron atoms and ions is

$$\frac{m_e}{4\pi r_1^2}\frac{v_1^2}{r_1} = \frac{e}{4\pi r_1^2}\frac{Ze}{4\pi\varepsilon_o r_1^2} - \frac{1}{4\pi r_1^2}\frac{\hbar^2}{m_p r_n^3}$$

$$r_1 = \frac{a_H}{Z}$$

where a_H is the radius of the hydrogen atom.

121. The system of claim 120, wherein from Maxwell's equations, the potential energy V, kinetic energy T, electric energy or binding energy E_{ele} are

$$V = \frac{-Ze^2}{4\pi\varepsilon_o r_1} = \frac{-Z^2e^2}{4\pi\varepsilon_o a_H} = -Z^2\ X\ 4.3675\ X\ 10^{-18}\ J = -Z^2\ X\ 27.2\ eV$$

$$T = \frac{Z^2e^2}{8\pi\varepsilon_o a_H} = Z^2\ X\ 13.59\ eV$$

$$T = E_{ele} = -\frac{1}{2}\varepsilon_o\int_{\infty}^{r_1}\mathbf{E}^2 dv \quad \text{where } \mathbf{E} = -\frac{Ze}{4\pi\varepsilon_o r^2}$$

$$E_{ele} = -\frac{Z^2e^2}{8\pi\varepsilon_o a_H} = -Z^2\ X\ 2.1786\ X\ 10^{-18}\ J = -Z^2\ X\ 13.598\ eV\,,$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

122. The system of claim 121, wherein the force balance equation solution of two electron atoms is a central force balance equation with the nonradiation condition is given by

$$\frac{m_e}{4\pi r_2^2}\frac{v_2^2}{r_2} = \frac{e}{4\pi r_2^2}\frac{(Z-1)e}{4\pi\varepsilon_o r_2^2} + \frac{1}{4\pi r_2^2}\frac{\hbar^2}{Zm_e r_2^3}\sqrt{s(s+1)}$$

which gives the radius of both electrons as

$$r_2 = r_1 = a_0\left(\frac{1}{Z-1} - \frac{\sqrt{s(s+1)}}{Z(Z-1)}\right);\ s = \frac{1}{2}.$$

123. The system of claim 122, wherein the ionization energy for helium, which has no electric field beyond r_1 is given by

$$Ionization\ Energy(He) = -E(electric) + E(magnetic)$$

where,

$$E(electric) = -\frac{(Z-1)e^2}{8\pi\varepsilon_o r_1}$$

$$E(magnetic) = \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_1^3}$$

For $3 \le Z$

$$Ionization\ Energy = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy.$$

124. The system of claim 123, wherein the electrons of multielectron atoms all exist as orbitspheres of discrete radii which are given by r_n of the radial Dirac delta function, $\delta(r-r_n)$.

125. The system of claim 124, wherein electron orbitspheres may be spin paired or unpaired depending on the force balance which applies to each electron wherein the electron configuration is a minimum of energy.

126. The system of claim 125, wherein the minimum energy configurations are given by solutions to Laplace's equation.

127. The system of claim 126, wherein the electrons of an atom with the same principal and ℓ quantum numbers align parallel until each of the m_ℓ levels are occupied, and then pairing occurs until each of the m_ℓ levels contain paired electrons.

128. The system of claim 127, wherein the electron configuration for one through twenty-electron atoms that achieves an energy minimum is: $1s < 2s < 2p < 3s < 3p < 4s$.

129. The system of claim 128, wherein the corresponding force balance of the central Coulombic, paramagnetic, and diamagnetic forces was derived for each n-electron atom that was solved for the radius of each electron.

130. The system of claim 129, wherein the central Coulombic force is that of a point charge at the origin since the electron charge-density functions are spherically symmetrical with a time dependence that is nonradiative.

131. The system of claim 130, wherein the ionization energies are obtained using the calculated radii in the determination of the Coulombic and any magnetic energies.

132. The system of claim 131, wherein the general equation for the radii of s electrons is given by

$$r_n = \frac{\dfrac{a_0\left(1+(C-D)\dfrac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)} \pm a_0\sqrt{\left(\dfrac{\left(1+(C-D)\dfrac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\dfrac{Z-n}{Z-(n-1)}\right]Er_m\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)}}}{2}$$

r_m *in units of* a_0

where positive root must be taken in order that $r_n > 0$;

Z is the nuclear charge, n is the number of electrons,

r_m is the radius of the proceeding filled shell(s) given by

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$$r_n = \frac{\frac{a_0\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_m}\right)} \pm a_0 \sqrt{\left(\frac{\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_m}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]Er_m\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_m}\right)}}}{2}$$

r_m *in units of* a_0

for the preceding s shell(s);

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}}}{2}$$

r_3 *in units of* a_0

for the 2p shell, and

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}}}{2}$$

r_{12} *in units of* a_0

for the 3p shell;

the parameter A corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic}$:

$$\mathbf{F}_{diamagnetic} = -\frac{\hbar^2}{4m_e r_3^2 r_1}\sqrt{s(s+1)}\mathbf{i}_r;$$

the parameter B corresponds to the paramagnetic force, $\mathbf{F}_{mag\ 2}$:

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_1 r_4^2}\sqrt{s(s+1)}\mathbf{i}_r;$$

the parameter C corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic\ 3}$:

$$\mathbf{F}_{diamagnetic\ 3} = -\frac{1}{Z}\frac{8\hbar^2}{m_e r_{11}^3}\sqrt{s(s+1)}\mathbf{i}_r;$$

the parameter D corresponds to the paramagnetic force, $\mathbf{F}_{mag}$:

$$\mathbf{F}_{mag} = \frac{1}{4\pi r_2^2}\frac{1}{Z}\frac{\hbar^2}{m_e r^3}\sqrt{s(s+1)}, \text{ and}$$

the parameter E corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic\ 2}$, due to a relativistic effect with an electric field for $r > r_n$:

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-3}{Z-2}\right]\frac{r_1\hbar^2}{m_e r_3^4}10\sqrt{3/4}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-11}{Z-10}\right]\left(1+\frac{\sqrt{2}}{2}\right)\frac{r_{10}\hbar^2}{m_e r_{11}^4}10\sqrt{s(s+1)}\mathbf{i}_r, \text{ and}$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)\frac{r_{18}\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r.$$

wherein the parameters of atoms filling the 1s, 2s, 3s, and 4s orbitals are

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of s Electrons (s state)	Diamag. Force Factor *A*	Paramag. Force Factor *B*	Diamag. Force Factor *C*	Paramag. Force Factor *D*	Diamag. Force Factor *E*
Neutral 1 e Atom *H*	$1s^1$	$^2S_{1/2}$	↑ 1s	0	0	0	0	0
Neutral 2 e Atom *He*	$1s^2$	$^1S_0$	↑ ↓ 1s	0	0	0	1	0
Neutral 3 e Atom *Li*	$2s^1$	$^2S_{1/2}$	↑ 2s	1	0	0	0	0
Neutral 4 e Atom *Be*	$2s^2$	$^1S_0$	↑ ↓ 2s	1	0	0	1	0
Neutral 11 e Atom *Na*	$1s^2 2s^2 2p^6 3s^1$	$^2S_{1/2}$	↑ 3s	1	0	8	0	0
Neutral 12 e Atom *Mg*	$1s^2 2s^2 2p^6 3s^2$	$^1S_0$	↑ ↓ 3s	1	3	12	1	0
Neutral 19 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$^2S_{1/2}$	↑ 4s	2	0	12	0	0

K								
Neutral	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	$^1S_0$	$\underline{\uparrow\downarrow}$					
20 e			4s	1	3	24	1	0
Atom								
Ca								
1 e Ion	$1s^1$	$^2S_{1/2}$	$\underline{\uparrow}$					
			1s	0	0	0	0	0
2 e Ion	$1s^2$	$^1S_0$	$\underline{\uparrow\downarrow}$					
			1s	0	0	0	1	0
3 e Ion	$2s^1$	$^2S_{1/2}$	$\underline{\uparrow}$					
			2s	1	0	0	0	1
4 e Ion	$2s^2$	$^1S_0$	$\underline{\uparrow\downarrow}$					
			2s	1	0	0	1	1
11 e Ion	$1s^2 2s^2 2p^6 3s^1$	$^2S_{1/2}$	$\underline{\uparrow}$					
			3s	1	4	8	0	$1+\frac{\sqrt{2}}{2}$
12 e Ion	$1s^2 2s^2 2p^6 3s^2$	$^1S_0$	$\underline{\uparrow\downarrow}$					
			3s	1	6	0	0	$1+\frac{\sqrt{2}}{2}$
19 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$^2S_{1/2}$	$\underline{\uparrow}$					
			4s	3	0	24	0	$2-\sqrt{2}$
20 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	$^1S_0$	$\underline{\uparrow\downarrow}$					
			4s	2	0	24	0	$2-\sqrt{2}$

133. The system of claim 132, with the radii, r_n, wherein the ionization energy for atoms having an outer s-shell are given by the negative of the electric energy, $E(electric)$, given by:

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}$$

except that minor corrections due to the magnetic energy must be included in cases wherein the s electron does not couple to p electrons as given by

$$Ionization\ Energy(He) = -E(electric) + E(magnetic)\left(1-\frac{1}{2}\left(\left(\frac{2}{3}\cos\frac{\pi}{3}\right)^2+\alpha\right)\right)$$

$$Ionization\ Energy = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy$$

$$E(ionization;\ Li) = \frac{(Z-2)e^2}{8\pi\varepsilon_o r_3} + \Delta E_{mag}$$
$$= 5.3178\ eV + 0.0860\ eV = 5.4038\ eV$$

$$E(Ionization) = E(Electric) + E_T$$

$$E(ionization;\ Be) = \frac{(Z-3)e^2}{8\pi\varepsilon_o r_4} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_4^3} + \Delta E_{mag}$$
$$= 8.9216\ eV + 0.03226\ eV + 0.33040\ eV = 9.28430\ eV$$

, and

$$E(Ionization) = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy - E_T$$

, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

134. The system of claim 133, wherein the radii and energies of the 2p electrons are solved using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z-n)e^2}{4\pi\varepsilon_o r_n^2}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r,$$

and the radii r_3 are given by

$$r_4 = r_3 = \frac{\left(\frac{a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o\sqrt{\frac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2}+4\frac{\left[\frac{Z-3}{Z-2}\right]r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}}\right)}{2}$$

r_1 in units of a_o

135. The system of claim 134, wherein the electric energy given by

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}$$

gives the corresponding ionization energies.

136. The system of claim 135, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^{n-4}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by:

$$r_1 = r_2 = a_o\left[\frac{1}{Z-1}-\frac{\sqrt{\frac{3}{4}}}{Z(Z-1)}\right];$$

two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by:

$$r_4 = r_3 = \frac{\left(\frac{a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o \sqrt{\frac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2} + 4\frac{\left[\frac{Z-3}{Z-2}\right] r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}} \right)}{2}$$

r_1 *in units of* a_o

and $n-4$ electrons in an orbitsphere with radius r_n given by

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}}}{2}$$

r_3 *in units of* a_0

the positive root must be taken in order that $r_n > 0$;

the parameter A corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic}$:

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!} \frac{\hbar^2}{4m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r ;$$

and the parameter B corresponds to the paramagnetic force, $\mathbf{F}_{mag\ 2}$:

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r ,$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z} \frac{4\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r , \text{ and}$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r$$

wherein the parameters of five through ten-electron atoms are

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of 2p Electrons (2p state)	Diamagnetic Force Factor A	Paramagnetic Force Factor B
Neutral 5 e Atom B	$1s^2 2s^2 2p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}\ \underline{\ }\ \underline{\ }$ 1 0 -1	2	0
Neutral 6 e Atom C	$1s^2 2s^2 2p^2$	$^3P_0$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\ }$ 1 0 -1	$\frac{2}{3}$	0
Neutral 7 e Atom N	$1s^2 2s^2 2p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{1}{3}$	1
Neutral 8 e Atom O	$1s^2 2s^2 2p^4$	$^3P_2$	$\underline{\uparrow\downarrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	1	2
Neutral 9 e Atom F	$1s^2 2s^2 2p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{2}{3}$	3
Neutral 10 e Atom Ne	$1s^2 2s^2 2p^6$	$^1S_0$	$\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}$ 1 0 -1	0	3
5 e Ion	$1s^2 2s^2 2p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}\ \underline{\ }\ \underline{\ }$ 1 0 -1	$\frac{5}{3}$	1
6 e Ion	$1s^2 2s^2 2p^2$	$^3P_0$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\ }$ 1 0 -1	$\frac{5}{3}$	4
7 e Ion	$1s^2 2s^2 2p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{5}{3}$	6

8 e Ion	$1s^2 2s^2 2p^4$	$^3P_2$	$\underline{\uparrow\downarrow}_1 \quad \underline{\uparrow}_0 \quad \underline{\uparrow}_{-1}$	$\frac{5}{3}$	6
9 e Ion	$1s^2 2s^2 2p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}_1 \quad \underline{\uparrow\downarrow}_0 \quad \underline{\uparrow}_{-1}$	$\frac{5}{3}$	9
10 e Ion	$1s^2 2s^2 2p^6$	$^1S_0$	$\underline{\uparrow\downarrow}_1 \quad \underline{\uparrow\downarrow}_0 \quad \underline{\uparrow\downarrow}_{-1}$	$\frac{5}{3}$	12

137. The system of claim 136, wherein the ionization energy for the boron atom is given by

$$E(ionization;\ B) = \frac{(Z-4)e^2}{8\pi\varepsilon_o r_5} + \Delta E_{mag}$$
$$= 8.147170901\ eV + 0.15548501\ eV = 8.30265592\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

138. The system of claim 137, wherein the ionization energies for the n-electron atoms having the radii, r_n ,are given by the negative of the electric energy, $E(electric)$, given by

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}.$$

139. The system of claim 138, wherein the radii of the 3p electrons are given using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z-n)e^2}{4\pi\varepsilon_o r_n^2}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\left(\frac{2}{3}+\frac{2}{3}+\frac{1}{3}\right)\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = -\left(\frac{5}{3}\right)\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = (4+4+4)\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = \frac{1}{Z}\frac{12\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{8\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

and the radii r_{12} are given by

$$r_{12} = \frac{\dfrac{a_0}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)} \pm a_0\sqrt{\left(\dfrac{1}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}}}{2}$$

r_{10} *in units of* a_0

140. The system of claim 139, wherein the ionization energies are given by electric energy given by:

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}.$$

141. The system of claim 140, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^6 3s^2 3p^{n-12}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by:

$$r_1 = r_2 = a_o \left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by:

$$r_4 = r_3 = \frac{\left(\frac{a_0 \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)} \pm a_o \sqrt{\frac{\left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)^2}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)^2} + 4 \frac{\left[\frac{Z-3}{Z-2} \right] r_1 10 \sqrt{\frac{3}{4}}}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)}} \right)}{2}$$

r_1 *in units of* a_o

three sets of paired indistinguishable electrons in an orbitsphere with radius r_{10} given by:

$$r_{10} = \frac{\frac{a_0}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)} \pm a_0 \sqrt{\frac{1}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)^2} + \frac{20\sqrt{3} \left(\left[\frac{Z-10}{Z-9} \right] \left(1 - \frac{\sqrt{2}}{2} \right) r_3 \right)}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)}}}{2}$$

r_3 *in units of* a_0

two indistinguishable spin-paired electrons in an orbitsphere with radius r_{12} given by:

$$r_{12} = \frac{\frac{a_0}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}}}{2}$$

r_{10} *in units of* a_0

and $n-12$ electrons in a 3p orbitsphere with radius r_n given by

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}}}{2}$$

r_{12} *in units of* a_0

where the positive root must be taken in order that $r_n > 0$;

the parameter A corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic}$:

$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$, and the parameter B corresponds to the paramagnetic force, $\mathbf{F}_{mag\,2}$:

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = (4+4+4)\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = \frac{1}{Z}\frac{12\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r, \text{ and}$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{8\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

wherein the parameters of thirteen through eighteen-electron atoms are

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of 3p Electrons (3p state)	Diamagnetic Force Factor *A*	Paramagnetic Force Factor *B*
Neutral 13 e Atom *Al*	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}_{1}\ \underline{\ }_{0}\ \underline{\ }_{-1}$	$\frac{11}{3}$	0
Neutral 14 e Atom *Si*	$1s^2 2s^2 2p^6 3s^2 3p^2$	$^3P_0$	$\underline{\uparrow}_{1}\ \underline{\uparrow}_{0}\ \underline{\ }_{-1}$	$\frac{7}{3}$	0
Neutral 15 e Atom *P*	$1s^2 2s^2 2p^6 3s^2 3p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}_{1}\ \underline{\uparrow}_{0}\ \underline{\uparrow}_{-1}$	$\frac{5}{3}$	2
Neutral 16 e Atom *S*	$1s^2 2s^2 2p^6 3s^2 3p^4$	$^3P_2$	$\underline{\uparrow\downarrow}_{1}\ \underline{\uparrow}_{0}\ \underline{\uparrow}_{-1}$	$\frac{4}{3}$	1
Neutral 17 e Atom *Cl*	$1s^2 2s^2 2p^6 3s^2 3p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}_{1}\ \underline{\uparrow\downarrow}_{0}\ \underline{\uparrow}_{-1}$	$\frac{2}{3}$	2
Neutral 18 e Atom *Ar*	$1s^2 2s^2 2p^6 3s^2 3p^6$	$^1S_0$	$\underline{\uparrow\downarrow}_{1}\ \underline{\uparrow\downarrow}_{0}\ \underline{\uparrow\downarrow}_{-1}$	$\frac{1}{3}$	4
13 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}_{1}\ \underline{\ }_{0}\ \underline{\ }_{-1}$	$\frac{5}{3}$	12

14 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^2$	$^3P_0$	$\underset{1}{\uparrow}$	$\underset{0}{\uparrow}$	$\underset{-1}{\quad}$	$\frac{1}{3}$	16
15 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^3$	$^4S^0_{3/2}$	$\underset{1}{\uparrow}$	$\underset{0}{\uparrow}$	$\underset{-1}{\uparrow}$	0	24
16 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^4$	$^3P_2$	$\underset{1}{\uparrow\downarrow}$	$\underset{0}{\uparrow}$	$\underset{-1}{\uparrow}$	$\frac{1}{3}$	24
17 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^5$	$^2P^0_{3/2}$	$\underset{1}{\uparrow\downarrow}$	$\underset{0}{\uparrow\downarrow}$	$\underset{-1}{\uparrow}$	$\frac{2}{3}$	32
18 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6$	$^1S_0$	$\underset{1}{\uparrow\downarrow}$	$\underset{0}{\uparrow\downarrow}$	$\underset{-1}{\uparrow\downarrow}$	0	40

142. The system of claim 141, wherein the ionization energies for the n-electron 3p atoms are given by electric energy given by:

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}.$$

143. The system of claim 142, wherein the ionization energy for the aluminum atom is given by

$$E(ionization;\ Al) = \frac{(Z-12)e^2}{8\pi\varepsilon_o r_{13}} + \Delta E_{mag}$$
$$= 5.95270\ eV + 0.031315\ eV = 5.98402\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

144. A system of claim 1 of computing the nature of bound atomic and atomic ionic electrons from physical solutions of the charge, mass, and current density functions of atoms

and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration, comprising:

processing means for processing and solving the equations for charge, mass, and current density functions of electron(s) in selected atoms or ions, wherein the equations are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration; and

output means for outputting the solutions of the charge, mass, and current density functions of the atoms and atomic ions.

145. A system of claim 1 comprising the steps of;

a.) inputting electron functions that are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration;

b.) inputting a trial electron configuration;

c.) inputting the corresponding centrifugal, Coulombic, diamagnetic and paramagnetic forces,

d.) forming the force balance equation comprising the centrifugal force equal to the sum of the Coulombic, diamagnetic and paramagnetic forces;

e.) solving the force balance equation for the electron radii;

f.) calculating the energy of the electrons using the radii and the corresponding electric and magnetic energies;

g.) repeating Steps a-f for all possible electron configurations, and

h.) outputting the lowest energy configuration and the corresponding electron radii for that configuration.

146. The system of claim 145, wherein the output is rendered using the electron functions.

147. The system of claim 146, wherein the electron functions are given by at least one of the group comprising:

$\ell = 0$

$$\rho(r,\theta,\phi,t) = \frac{e}{8\pi r^2}[\delta(r-r_n)]\left[Y_0^0(\theta,\phi)+Y_t^m(\theta,\phi)\right]$$

$\ell \neq 0$

$$\rho(r,\theta,\phi,t) = \frac{e}{4\pi r^2}[\delta(r-r_n)]\left[Y_0^0(\theta,\phi) + \mathrm{Re}\left\{Y_\ell^m(\theta,\phi)e^{i\omega_n t}\right\}\right]$$

where $Y_\ell^m(\theta,\phi)$ are the spherical harmonic functions that spin about the z-axis with angular frequency ω_n with $Y_0^0(\theta,\phi)$ the constant function. $\mathrm{Re}\left\{Y_\ell^m(\theta,\phi)e^{i\omega_n t}\right\} = P_\ell^m(\cos\theta)\cos\left(m\phi + \omega_n' t\right)$ where to keep the form of the spherical harmonic as a traveling wave about the z-axis, $\omega_n' = m\omega_n$.

148. The system of claim 147, wherein the forces are given by at least one of the group comprising:

$$\mathbf{F}_{ele} = \frac{(Z-n)e^2}{4\pi\varepsilon_o r_n^2}\mathbf{i}_r$$

$$\mathbf{F}_{ele} = \frac{(Z-(n-1))e^2}{4\pi\varepsilon_o r_n^2}\mathbf{i}_r$$

$$\mathbf{F}_{mag} = \frac{1}{4\pi r_2^{\,2}}\frac{1}{Z}\frac{\hbar^2}{m_e r^3}\sqrt{s(s+1)}$$

$$\mathbf{F}_{diamagnetic} = -\frac{\hbar^2}{4m_e r_3^2 r_1}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\left(\frac{2}{3}+\frac{2}{3}+\frac{1}{3}\right)\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = -\left(\frac{5}{3}\right)\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-3}{Z-2}\right]\frac{r_1\hbar^2}{m_e r_3^4}10\sqrt{3/4}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-11}{Z-10}\right]\left(1+\frac{\sqrt{2}}{2}\right)\frac{r_{10}\hbar^2}{m_e r_{11}^4}10\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)\frac{r_{18}\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 3} = -\frac{1}{Z}\frac{8\hbar^2}{m_e r_{11}^{\ 3}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_1 r_4^2}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = (4+4+4)\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = \frac{1}{Z}\frac{12\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r, \text{ and}$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{8\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

149. The system of claim 148, wherein the radii are given by at least one of the group comprising:

$$r_1 = r_2 = a_o\left[\frac{1}{Z-1}-\frac{\sqrt{\frac{3}{4}}}{Z(Z-1)}\right]$$

$$r_4 = r_3 = \frac{\dfrac{a_0\left(1-\dfrac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o \sqrt{\dfrac{\left(1-\dfrac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2} + 4\dfrac{\left[\frac{Z-3}{Z-2}\right] r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}}}{2}$$

r_1 in units of a_o

$$r_n = \frac{\dfrac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)} \pm a_0 \sqrt{\left(\dfrac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}}}{2}$$

r_3 in units of a_0

$$r_{10} = \frac{\dfrac{a_0}{\left((Z-9)-\left(\frac{5}{24}-\frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)} \pm a_0 \sqrt{\left(\dfrac{1}{\left((Z-9)-\left(\frac{5}{24}-\frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\frac{Z-10}{Z-9}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-9)-\left(\frac{5}{24}-\frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)}}}{2}$$

r_3 in units of a_0

$$r_{11} = \frac{a_0\left(1+\frac{8}{Z}\sqrt{\frac{3}{4}}\right)}{(Z-10)-\frac{\sqrt{\frac{3}{4}}}{4r_{10}}},\ r_{10} \text{ in units of } a_0$$

$$r_{12} = \frac{\frac{a_0}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}}}{2}$$

r_{10} *in units of* a_0

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}}}{2}$$

r_{12} *in units of* a_0

$$r_n = \frac{\frac{a_0\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_m}\right)} \pm a_0 \sqrt{\left(\frac{\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_m}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]Er_m\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_m}\right)}}}{2}$$

r_m *in units of* a_0

150. The system of claim 149, wherein the electric energy of each electron of radius r_n is given by at least one of the group comprising:

$$E(electric) = -\frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}$$

$$Ionization\ Energy(He) = -E(electric) + E(magnetic)\left(1-\frac{1}{2}\left(\left(\frac{2}{3}\cos\frac{\pi}{3}\right)^2+\alpha\right)\right)$$

$$Ionization\ Energy = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy$$

$$E(Ionization) = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy - E_T$$

$$E(ionization;\ Li) = \frac{(Z-2)e^2}{8\pi\varepsilon_o r_3} + \Delta E_{mag}$$
$$= 5.3178\ eV + 0.0860\ eV = 5.4038\ eV$$

$$E(ionization;\ B) = \frac{(Z-4)e^2}{8\pi\varepsilon_o r_5} + \Delta E_{mag}$$
$$= 8.147170901\ eV + 0.15548501\ eV = 8.30265592\ eV$$

$$E(ionization;\ Be) = \frac{(Z-3)e^2}{8\pi\varepsilon_o r_4} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_4^3} + \Delta E_{mag}$$
$$= 8.9216\ eV + 0.03226\ eV + 0.33040\ eV = 9.28430\ eV$$

$$E(ionization;\ Na) = -Electric\ Energy = \frac{(Z-10)e^2}{8\pi\varepsilon_o r_{11}} = 5.12592\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

151. The system of claim 150, wherein the radii of s electrons are given by

$$r_n = \frac{\dfrac{a_0\left(1+(C-D)\dfrac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)} \pm a_0 \sqrt{\left(\dfrac{\left(1+(C-D)\dfrac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\dfrac{Z-n}{Z-(n-1)}\right]Er_m\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)}}}{2}$$

r_m *in units of* a_0

where positive root must be taken in order that $r_n > 0$;

Z is the nuclear charge, n is the number of electrons,

r_m is the radius of the proceeding filled shell(s) given by

$$r_n = \frac{\dfrac{a_0\left(1+(C-D)\dfrac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)} \pm a_0 \sqrt{\left(\dfrac{\left(1+(C-D)\dfrac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\dfrac{Z-n}{Z-(n-1)}\right]Er_m\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_m}\right)}}}{2}$$

r_m *in units of* a_0

for the preceding s shell(s);

$$r_n = \frac{\dfrac{a_0}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_3}\right)} \pm a_0 \sqrt{\left(\dfrac{1}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_3}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\dfrac{Z-n}{Z-(n-1)}\right]\left(1-\dfrac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_3}\right)}}}{2}$$

r_3 *in units of* a_0

for the 2p shell, and

$$r_n = \frac{\dfrac{a_0}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_{12}}\right)} \pm a_0 \sqrt{\left(\dfrac{1}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_{12}}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\dfrac{Z-n}{Z-(n-1)}\right]\left(1-\dfrac{\sqrt{2}}{2}+\dfrac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\dfrac{A}{8}-\dfrac{B}{2Z}\right)\dfrac{\sqrt{3}}{r_{12}}\right)}}}{2}$$

r_{12} *in units of* a_0

for the 3p shell;

the parameter A corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic}$:

$$\mathbf{F}_{diamagnetic} = -\frac{\hbar^2}{4m_e r_3^2 r_1}\sqrt{s(s+1)}\mathbf{i}_r;$$

the parameter B corresponds to the paramagnetic force, $\mathbf{F}_{mag\ 2}$:

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_1 r_4^2}\sqrt{s(s+1)}\mathbf{i}_r;$$

the parameter C corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic\ 3}$:

$$\mathbf{F}_{diamagnetic\ 3} = -\frac{1}{Z}\frac{8\hbar^2}{m_e r_{11}^3}\sqrt{s(s+1)}\mathbf{i}_r;$$

the parameter D corresponds to the paramagnetic force, $\mathbf{F}_{mag}$:

$$\mathbf{F}_{mag} = \frac{1}{4\pi r_2^2}\frac{1}{Z}\frac{\hbar^2}{m_e r^3}\sqrt{s(s+1)}\,, \text{ and}$$

the parameter E corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic\ 2}$, due to a relativistic effect with an electric field for $r > r_n$:

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-3}{Z-2}\right]\frac{r_1\hbar^2}{m_e r_3^4}10\sqrt{3/4}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-11}{Z-10}\right]\left(1+\frac{\sqrt{2}}{2}\right)\frac{r_{10}\hbar^2}{m_e r_{11}^4}10\sqrt{s(s+1)}\mathbf{i}_r\text{, and}$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)\frac{r_{18}\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r\,.$$

wherein the parameters of atoms filling the 1s, 2s, 3s, and 4s orbitals are

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of s Electrons (s state)	Dia mag. Force Factor *A*	Para mag. Force Factor *B*	Dia mag. Force Factor *C*	Para mag. Force Factor *D*	Diamag. Force Factor *E*
Neutral 1 e Atom *H*	$1s^1$	$^2S_{1/2}$	↑ 1s	0	0	0	0	0
Neutral 2 e Atom *He*	$1s^2$	$^1S_0$	↑ ↓ 1s	0	0	0	1	0
Neutral 3 e Atom *Li*	$2s^1$	$^2S_{1/2}$	↑ 2s	1	0	0	0	0
Neutral 4 e Atom *Be*	$2s^2$	$^1S_0$	↑ ↓ 2s	1	0	0	1	0
Neutral 11 e Atom *Na*	$1s^2 2s^2 2p^6 3s^1$	$^2S_{1/2}$	↑ 3s	1	0	8	0	0
Neutral 12 e Atom *Mg*	$1s^2 2s^2 2p^6 3s^2$	$^1S_0$	↑ ↓ 3s	1	3	12	1	0

Neutral 19 e Atom *K*	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$^2S_{1/2}$	↑ 4s	2	0	12	0	0
Neutral 20 e Atom *Ca*	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	$^1S_0$	↑ ↓ 4s	1	3	24	1	0
1 e Ion	$1s^1$	$^2S_{1/2}$	↑ 1s	0	0	0	0	0
2 e Ion	$1s^2$	$^1S_0$	↑ ↓ 1s	0	0	0	1	0
3 e Ion	$2s^1$	$^2S_{1/2}$	↑ 2s	1	0	0	0	1
4 e Ion	$2s^2$	$^1S_0$	↑ ↓ 2s	1	0	0	1	1
11 e Ion	$1s^2 2s^2 2p^6 3s^1$	$^2S_{1/2}$	↑ 3s	1	4	8	0	$1+\frac{\sqrt{2}}{2}$
12 e Ion	$1s^2 2s^2 2p^6 3s^2$	$^1S_0$	↑ ↓ 3s	1	6	0	0	$1+\frac{\sqrt{2}}{2}$
19 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$^2S_{1/2}$	↑ 4s	3	0	24	0	$2-\sqrt{2}$
20 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	$^1S_0$	↑ ↓ 4s	2	0	24	0	$2-\sqrt{2}$

152. The system of claim 151, with the radii, r_n, wherein the ionization energy for atoms having an outer s-shell are given by the negative of the electric energy, $E(electric)$, given by:

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}$$

except that minor corrections due to the magnetic energy must be included in cases wherein the s electron does not couple to p electrons as given by

$$Ionization\ Energy(He) = -E(electric) + E(magnetic)\left(1-\frac{1}{2}\left(\left(\frac{2}{3}\cos\frac{\pi}{3}\right)^2+\alpha\right)\right)$$

$$Ionization\ Energy = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy$$

$$E(ionization;\ Li) = \frac{(Z-2)e^2}{8\pi\varepsilon_o r_3} + \Delta E_{mag}$$
$$= 5.3178\ eV + 0.0860\ eV = 5.4038\ eV$$

$$E(Ionization) = E(Electric) + E_T$$

$$E(ionization;\ Be) = \frac{(Z-3)e^2}{8\pi\varepsilon_o r_4} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_4^3} + \Delta E_{mag}$$
$$= 8.9216\ eV + 0.03226\ eV + 0.33040\ eV = 9.28430\ eV$$

, and

$$E(Ionization) = -Electric\ Energy - \frac{1}{Z}Magnetic\ Energy - E_T$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

153. The system of claim 152, wherein the radii and energies of the 2p electrons are solved using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z-n)e^2}{4\pi\varepsilon_o r_n^2}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r,$$

and the radii r_3 are given by

$$r_4 = r_3 = \frac{\left(\frac{a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o\sqrt{\frac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2}+4\frac{\left[\frac{Z-3}{Z-2}\right]r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}}\right)}{2}$$

r_1 in units of a_o

154. The system of claim 153, wherein the electric energy given by

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}$$

gives the corresponding ionization energies.

155. The system of claim 154, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^{n-4}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by:

$$r_1 = r_2 = a_o\left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)}\right];$$

two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by:

$$r_4 = r_3 = \frac{\left(\frac{a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o\sqrt{\frac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2} + 4\frac{\left[\frac{Z-3}{Z-2}\right]r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}}\right)}{2}$$

r_1 *in units of* a_o

and $n-4$ electrons in an orbitsphere with radius r_n given by

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)} \pm a_0\sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_3}\right)}}}{2};$$

r_3 *in units of* a_0

the positive root must be taken in order that $r_n > 0$;

the parameter A corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic}$:

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!} \frac{\hbar^2}{4m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r;$$

and the parameter B corresponds to the paramagnetic force, $\mathbf{F}_{mag\ 2}$:

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r,$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z} \frac{4\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r, \text{ and}$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)}\mathbf{i}_r.$$

wherein the parameters of five through ten-electron atoms are

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of 2p Electrons (2p state)	Diamagnetic Force Factor A	Paramagnetic Force Factor B
Neutral 5 e Atom B	$1s^2 2s^2 2p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}\ \underline{\ \ }\ \underline{\ \ }$ 1 0 -1	2	0
Neutral 6 e Atom C	$1s^2 2s^2 2p^2$	$^3P_0$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\ \ }$ 1 0 -1	$\frac{2}{3}$	0
Neutral 7 e Atom N	$1s^2 2s^2 2p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{1}{3}$	1
Neutral 8 e Atom O	$1s^2 2s^2 2p^4$	$^3P_2$	$\underline{\uparrow\downarrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	1	2
Neutral 9 e Atom F	$1s^2 2s^2 2p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{2}{3}$	3
Neutral 10 e Atom Ne	$1s^2 2s^2 2p^6$	$^1S_0$	$\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}$ 1 0 -1	0	3
5 e Ion	$1s^2 2s^2 2p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}\ \underline{\ \ }\ \underline{\ \ }$ 1 0 -1	$\frac{5}{3}$	1
6 e Ion	$1s^2 2s^2 2p^2$	$^3P_0$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\ \ }$ 1 0 -1	$\frac{5}{3}$	4
7 e Ion	$1s^2 2s^2 2p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{5}{3}$	6

8 e Ion	$1s^2 2s^2 2p^4$	$^3P_2$	$\underline{\uparrow\downarrow}_{1}\ \underline{\uparrow}_{0}\ \underline{\uparrow}_{-1}$	$\frac{5}{3}$	6
9 e Ion	$1s^2 2s^2 2p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}_{1}\ \underline{\uparrow\downarrow}_{0}\ \underline{\uparrow}_{-1}$	$\frac{5}{3}$	9
10 e Ion	$1s^2 2s^2 2p^6$	$^1S_0$	$\underline{\uparrow\downarrow}_{1}\ \underline{\uparrow\downarrow}_{0}\ \underline{\uparrow\downarrow}_{-1}$	$\frac{5}{3}$	12

156. The system of claim 155, wherein the ionization energy for the boron atom is given by

$$E(ionization;\ B) = \frac{(Z-4)e^2}{8\pi\varepsilon_o r_5} + \Delta E_{mag}$$
$$= 8.147170901\ eV + 0.15548501\ eV = 8.30265592\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

157. The system of claim 156, wherein the ionization energies for the n-electron atoms having the radii, r_n ,are given by the negative of the electric energy, $E(electric)$, given by

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}.$$

158. The system of claim 157, wherein the radii of the 3p electrons are given using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z-n)e^2}{4\pi\varepsilon_o r_n^2}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\left(\frac{2}{3}+\frac{2}{3}+\frac{1}{3}\right)\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = -\left(\frac{5}{3}\right)\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = (4+4+4)\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = \frac{1}{Z}\frac{12\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\,2} = \frac{1}{Z}\frac{8\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

and the radii r_{12} are given by

$$r_{12} = \frac{\dfrac{a_0}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)} \pm a_0\sqrt{\left(\dfrac{1}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}}}{2}$$

r_{10} *in units of* a_0

159. The system of claim 158, wherein the ionization energies are given by electric energy given by:

$$E(Ionization) = -Electric\ Energy = \frac{(Z-(n-1))e^2}{8\pi\varepsilon_o r_n}.$$

160. The system of claim 159, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^6 3s^2 3p^{n-12}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by:

$$r_1 = r_2 = a_o \left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by:

$$r_4 = r_3 = \frac{\left(\frac{a_0 \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)} \pm a_o \sqrt{\frac{\left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)^2}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)^2} + 4 \frac{\left[\frac{Z-3}{Z-2} \right] r_1 10 \sqrt{\frac{3}{4}}}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)}} \right)}{2}$$

r_1 *in units of* a_o

three sets of paired indistinguishable electrons in an orbitsphere with radius r_{10} given by:

$$r_{10} = \frac{\frac{a_0}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)} \right)^2 + \frac{20\sqrt{3} \left(\left[\frac{Z-10}{Z-9} \right] \left(1 - \frac{\sqrt{2}}{2} \right) r_3 \right)}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)}}}{2}$$

r_3 *in units of* a_0

two indistinguishable spin-paired electrons in an orbitsphere with radius r_{12} given by:

$$r_{12} = \frac{\frac{a_0}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}}}{2}$$

r_{10} *in units of* a_0

and $n-12$ electrons in a 3p orbitsphere with radius r_n given by

$$r_n = \frac{\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)} \pm a_0 \sqrt{\left(\frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}}}{2}$$

r_{12} *in units of* a_0

where the positive root must be taken in order that $r_n > 0$;

the parameter A corresponds to the diamagnetic force, $\mathbf{F}_{diamagnetic}$:

$\mathbf{F}_{diamagnetic} = -\sum_m \frac{(\ell+|m|)!}{(2\ell+1)(\ell-|m|)!}\frac{\hbar^2}{4m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$, and the parameter B corresponds to the paramagnetic force, $\mathbf{F}_{mag\ 2}$:

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = (4+4+4)\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r = \frac{1}{Z}\frac{12\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{4\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r, \text{ and}$$

$$\mathbf{F}_{mag\ 2} = \frac{1}{Z}\frac{8\hbar^2}{m_e r_n^2 r_{12}}\sqrt{s(s+1)}\mathbf{i}_r,$$

wherein the parameters of thirteen to eighteen-electron atoms are

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of 3p Electrons (3p state)	Diamagnetic Force Factor *A*	Paramagnetic Force Factor *B*
Neutral 13 e Atom *Al*	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}\ \underline{\ }\ \underline{\ }$ 1 0 -1	$\frac{11}{3}$	0
Neutral 14 e Atom *Si*	$1s^2 2s^2 2p^6 3s^2 3p^2$	$^3P_0$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\ }$ 1 0 -1	$\frac{7}{3}$	0
Neutral 15 e Atom *P*	$1s^2 2s^2 2p^6 3s^2 3p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{5}{3}$	2
Neutral 16 e Atom *S*	$1s^2 2s^2 2p^6 3s^2 3p^4$	$^3P_2$	$\underline{\uparrow\downarrow}\ \underline{\uparrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{4}{3}$	1
Neutral 17 e Atom *Cl*	$1s^2 2s^2 2p^6 3s^2 3p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow}$ 1 0 -1	$\frac{2}{3}$	2
Neutral 18 e Atom *Ar*	$1s^2 2s^2 2p^6 3s^2 3p^6$	$^1S_0$	$\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}$ 1 0 -1	$\frac{1}{3}$	4
13 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^2P^0_{1/2}$	$\underline{\uparrow}\ \underline{\ }\ \underline{\ }$ 1 0 -1	$\frac{5}{3}$	12

14 e Ion $1s^2 2s^2 2p^6 3s^2 3p^2$	$^3P_0$	$\underline{\uparrow}$ 1	$\underline{\uparrow}$ 0	$\underline{\quad}$ -1	$\frac{1}{3}$	16
15 e Ion $1s^2 2s^2 2p^6 3s^2 3p^3$	$^4S^0_{3/2}$	$\underline{\uparrow}$ 1	$\underline{\uparrow}$ 0	$\underline{\uparrow}$ -1	0	24
16 e Ion $1s^2 2s^2 2p^6 3s^2 3p^4$	$^3P_2$	$\underline{\uparrow\downarrow}$ 1	$\underline{\uparrow}$ 0	$\underline{\uparrow}$ -1	$\frac{1}{3}$	24
17 e Ion $1s^2 2s^2 2p^6 3s^2 3p^5$	$^2P^0_{3/2}$	$\underline{\uparrow\downarrow}$ 1	$\underline{\uparrow\downarrow}$ 0	$\underline{\uparrow}$ -1	$\frac{2}{3}$	32
18 e Ion $1s^2 2s^2 2p^6 3s^2 3p^6$	$^1S_0$	$\underline{\uparrow\downarrow}$ 1	$\underline{\uparrow\downarrow}$ 0	$\underline{\uparrow\downarrow}$ -1	0	40

161. The system of claim 160 wherein the bond comprises a H_2-type MO with two paired electron wherein the formation of the H_2-type MO by the contribution of an electron from each participating atom results in a diamagnetic force between the remaining atomic electrons and the H_2-type MO which causes the H_2-type MO to move to greater principal axes than would result with the Coulombic force alone.

162. The system of claim 161 wherein the integer increase of the central field and the resulting increased Coulombic as well as magnetic central forces on the remaining atomic electrons of each atom decrease the radius of the corresponding shell such that the energy minimum is achieved that is lower than that of the reactant atoms.

163. The system of claim 162 wherein the general equation for the central Coulomb force on the outer-most shell (nth where $n = Z - 1$) electron due to the nucleus and the inner electrons is given by:

$$\mathbf{F}_{ele} = \frac{2e^2}{4\pi\varepsilon_0 r_n^2}\mathbf{i}_r$$

for $r > r_{n-1}$.

164. The system of claim 163 wherein the general equation for $\mathbf{F}_{diamagnetic}$ due to the p-orbital contribution is given by

$$\mathbf{F}_{diamagnetic} = -A\frac{\hbar^2}{12m_e r_n^2 r_3}\sqrt{\frac{3}{4}}\mathbf{i}_r$$

165. The system of claim 164 wherein the general equation for $\mathbf{F}_{mag\ 2}$ is given by

$$\mathbf{F}_{mag\ 2} = B\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

166. The system of claim 165 wherein the general equation for $\mathbf{F}_{diamagnetic\ 2}$ due to the binding of the p-orbital electron having an electric field of +1 outside of its radius is given by

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{1}{2}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r$$

167. The system of claim 166 wherein the general equation for $\mathbf{F}_{mag\ 3}$, due to the contribution of a $2p$ electron from each binding atom in the formation of the σ MO that gives rise to a paramagnetic force on the remaining two $2p$ electrons that pair, is given by

$$\mathbf{F}_{mag\ 3} = C\frac{\hbar^2}{4m_e r_n^3}\sqrt{s(s+1)}\mathbf{i}_r$$

168. The system of claim 167 wherein the parameters A, B, and C are zero or a positive integer such that the resulting energy of the molecule is minimized and the electron angular momentum is conserved in the formation of the specie.

169. The system of claim 168 wherein the radius of the $2p$ shell is calculated by equating the outward centrifugal force to the sum of the electric and diamagnetic and paramagnetic forces:

$$\frac{m_e v_n^2}{r_n} = \left(\begin{array}{l} \frac{2e^2}{4\pi\varepsilon_0 r_n^2} - A\frac{\hbar^2}{12 m_e r_n^2 r_3}\sqrt{s(s+1)} + B\frac{\hbar^2}{Z m_e r_n^2 r_3}\sqrt{s(s+1)} \\ -\left[\frac{1}{2}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{r_n^4 m_e}10\sqrt{s(s+1)} + C\frac{\hbar^2}{4 m_e r_n^3}\sqrt{s(s+1)} \end{array} \right)$$

170. The system of claim 169 wherein the radius of the $2p$ shell is calculated by equating the outward centrifugal force to the sum of the electric and diamagnetic and paramagnetic forces where the velocity given by $v_n = \frac{\hbar}{m_e r_n}$ and $s = \frac{1}{2}$ gives:

$$\frac{\hbar^2}{m_e r_n^3} - C\frac{\hbar^2}{4 m_e r_n^3}\sqrt{\frac{3}{4}} = \frac{2e^2}{4\pi\varepsilon_0 r_n^2} - A\frac{\hbar^2}{12 m_e r_n^2 r_3}\sqrt{\frac{3}{4}} + B\frac{\hbar^2}{Z m_e r_6^2 r_3}\sqrt{\frac{3}{4}} - \left[\frac{1}{2}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{r_n^4 m_e}10\sqrt{\frac{3}{4}}$$

171. The system of claim 170 wherein the general equation for the radius of the shell of the remaining electrons is given by

$$r_6 = \frac{\frac{a_0\left(1-C\frac{\sqrt{3}}{8}\right)}{\left(2-\left(\frac{A}{12}-\frac{B}{Z}\right)\frac{\sqrt{3}}{2r_3}\right)} \pm a_0\sqrt{\left(\frac{1-C\frac{\sqrt{3}}{8}}{\left(2-\left(\frac{A}{12}-\frac{B}{Z}\right)\frac{\sqrt{3}}{2r_3}\right)}\right)^2 + \frac{20\sqrt{3}\left(\left[\frac{1}{2}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left(2-\left(\frac{A}{12}-\frac{B}{Z}\right)\frac{\sqrt{3}}{2r_3}\right)}}}{2}$$

r_3 *in units of* a_0

172. The system of claim 171 wherein the radii r_3 are given by

$$r_4 = r_3 = \frac{\left(\frac{a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o \sqrt{\frac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2} + 4\frac{\left[\frac{Z-3}{Z-2}\right] r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}} \right)}{2}$$

r_1 *in units of* a_o

173. The system of claim 172, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^{n-4}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by:

$$r_1 = r_2 = a_o\left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)}\right];$$

and two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by:

$$r_4 = r_3 = \frac{\left(a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right) \Big/ \left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right) \right) \pm a_o \sqrt{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2 \Big/ \left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2 + 4\frac{\left[\frac{Z-3}{Z-2}\right] r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}}}{2}$$

r_1 *in units of* a_o

174. The system of claim 173 wherein the sum $E_T\left(molecule, AOs\right)$ of the Coulombic energy change of the AO electrons of both atoms of a bond is given by using the initial radius r_n of each atom and the final radius r_{n-1} of the binding shell of each atom and by considering that the central Coulombic field decreases by an integer for each successive electron of the shell:

$$E_T\left(molecule, AOs\right) = \sum_{m=n_1-3}^{n_1-2} \frac{(Z-m)e^2}{8\pi\varepsilon_0}\left(\frac{1}{r_{n_1-1}}-\frac{1}{r_{n_1}}\right) + \sum_{m=n_2-3}^{n_2-2} \frac{(Z-m)e^2}{8\pi\varepsilon_0}\left(\frac{1}{r_{n_2-1}}-\frac{1}{r_{n_2}}\right)$$

where the subscript designates atom 1 and atom 2 of the bond.

175. The system of claim 174 wherein the forces on the electrons of the MO are the Coulombic force:

$$\mathbf{F}_{Coulomb} = \frac{e^2}{8\pi\varepsilon_0 ab^2} D\mathbf{i}_\xi ;$$

the spin pairing force:

$$\mathbf{F}_{spin-pairing} = \frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi$$

the diamagnetic force:

$$\mathbf{F}_{diamagneticMO1} = -\frac{n_e \hbar^2}{4m_e a^2 b^2} D\mathbf{i}_\xi$$

where n_e is the total number of electrons that interact with the binding σ-MO electron, the force on the pairing electron of the σ MO:

$$\mathbf{F}_{diamagneticMO2} = -\frac{1}{Z}\frac{|L|\hbar}{2m_e a^2 b^2} D\mathbf{i}_\xi$$

where $|L|$ is the magnitude of the angular momentum of each atom at a focus that is the source of the diamagnetism at the σ-MO, and the centrifugal force:

$$\mathbf{F}_{centrifugalMO} = -\frac{\hbar^2}{m_e a^2 b^2} D\mathbf{i}_\xi$$, wherein the force balance of the centrifugal force equated to the Coulombic and magnetic forces is solved for the length of the semimajor axis.

176. The system of claim 175 wherein the force balance equation for the σ-MO with $n_e = 2$ and $|L| = \hbar$ is

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 ab^2} D + \frac{\hbar^2}{2m_e a^2 b^2} D - \left(1 + \frac{1}{Z}\right)\frac{\hbar^2}{2m_e a^2 b^2} D$$

$$a = \left(2 + \frac{1}{Z}\right) a_0$$

177. The system of claim 176 wherein the force balance equation for the σ-MO with $n_e = 2$ and $|L| = \sqrt{\frac{3}{4}}\hbar$ is

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 ab^2} D + \frac{\hbar^2}{2m_e a^2 b^2} D - \left(\frac{3}{2} + \frac{\sqrt{\frac{3}{4}}}{Z}\right)\frac{\hbar^2}{2m_e a^2 b^2} D$$

$$a = \left(\frac{5}{2} + \frac{\sqrt{\frac{3}{4}}}{Z}\right) a_0$$

178. The system of claim 177 wherein the force balance equation for the σ-MO $n_e = 2$, and $|L| = \hbar$:

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 a b^2} D + \frac{\hbar^2}{2 m_e a^2 b^2} D - \left(\frac{5}{2} + \frac{1}{2Z}\right) \frac{\hbar^2}{2 m_e a^2 b^2} D$$

$$a = \left(\frac{7}{2} + \frac{1}{2Z}\right) a_0$$

179. The system of claim 178 wherein the Coulombic force is

$$\mathbf{F}_{Coulomb} = \frac{e^2}{8\pi\varepsilon_0 a b^2} D \mathbf{i}_\xi ;$$

the spin pairing force is

$$\mathbf{F}_{spin-pairing} = \frac{\hbar^2}{2 m_e a^2 b^2} D \mathbf{i}_\xi$$

the force on the electrons of the MO due to two paired electrons in at least one shell with $n_e = 2$ is

$$\mathbf{F}_{diamagneticMO1} = -\frac{\hbar^2}{2 m_e a^2 b^2} D \mathbf{i}_\xi ;$$

the force $\mathbf{F}_{diamagneticMO2}$ is given by the sum of the contributions over the components of angular momentum $|L|$ of the atoms at the foci acting on the electrons of the σ-MO:

$$\mathbf{F}_{diamagneticMO2} = -\sum_{i,j} \frac{|L_i| \hbar}{Z_j 2 m_e a^2 b^2} D \mathbf{i}_\xi , \text{ and}$$

the centrifugal force is

$$\mathbf{F}_{centrifugalMO} = -\frac{\hbar^2}{m_e a^2 b^2} D \mathbf{i}_\xi .$$

180. The system of claim 179 wherein the force balance equation for the σ-MO of the carbon nitride radical comprising carbon with charge $Z_1 = 6$ and $|L_1| = \hbar$ and $|L_2| = \sqrt{\frac{3}{4}}\hbar$ and nitrogen with $Z_2 = 7$ and $|L_3| = \hbar$ is

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 ab^2} D + \frac{\hbar^2}{2m_e a^2 b^2} D - \left(1 + \frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{1}{Z_2}\right) \frac{\hbar^2}{2m_e a^2 b^2} D$$

$$a = \left(2 + \frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{1}{Z_2}\right) a_0$$

181. The system of claim 180 wherein the Coulombic force is

$$\mathbf{F}_{Coulomb} = \frac{e^2}{8\pi\varepsilon_0 ab^2} D\mathbf{i}_\xi ;$$

the spin pairing force is

$$\mathbf{F}_{spin-pairing} = \frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi$$

the force on the electrons of the MO due to two paired electrons in at least one shell with $n_{e^-} = 2$ is

$$\mathbf{F}_{diamagneticMO1} = -\frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi ;$$

the force $\mathbf{F}_{diamagneticMO2}$ is given by the sum of the contributions over the components of angular momentum $|L|$ of the atoms at the foci acting on the electrons of the σ-MO:

$$\mathbf{F}_{diamagneticMO2} = -\sum_{i,j} \frac{|L_i|\hbar}{Z_j 2m_e a^2 b^2} D\mathbf{i}_\xi , \text{ and}$$

the centrifugal force is

$$\mathbf{F}_{centrifugalMO} = -\frac{\hbar^2}{m_e a^2 b^2} D\mathbf{i}_\xi .$$

182. The system of claim 181 wherein the force balance equation for the σ-MO of the carbon nitride radical comprising carbon with charge $Z_1 = 6$ and $|L_1| = \hbar$ and $|L_2| = \sqrt{\frac{3}{4}}\hbar$ and nitrogen with $Z_2 = 7$ and $|L_3| = \hbar$ is

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 a b^2} D + \frac{\hbar^2}{2 m_e a^2 b^2} D - \left(1 + \frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{1}{Z_2}\right) \frac{\hbar^2}{2 m_e a^2 b^2} D$$

$$a = \left(2 + \frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{1}{Z_2}\right) a_0$$

183. The system of claim 182 wherein the Coulombic force is

$$\mathbf{F}_{Coulomb} = \frac{e^2}{8\pi\varepsilon_0 a b^2} D \mathbf{i}_\xi ;$$

the spin pairing force is

$$\mathbf{F}_{spin-pairing} = \frac{\hbar^2}{2 m_e a^2 b^2} D \mathbf{i}_\xi$$

the force on the electrons of the MO due to two paired electrons in at least one shell with $n_e = 2$ is

$$\mathbf{F}_{diamagneticMO1} = -\frac{\hbar^2}{2 m_e a^2 b^2} D \mathbf{i}_\xi ;$$

the force $\mathbf{F}_{diamagneticMO2}$ is given by the sum of the contributions over the components of angular momentum $|L|$ of the atoms at the foci acting on the electrons of the σ-MO, and the sum of the contributions from atom 1 with $Z = Z_1$ and atom 2 with $Z = Z_2$ with $|L_i| = \hbar$ is

$$\mathbf{F}_{diamagneticMO2} = -\left(\frac{1}{Z_1} + \frac{1}{Z_2}\right) \frac{\hbar^2}{2 m_e a^2 b^2} D \mathbf{i}_\xi , \text{ and}$$

the centrifugal force is

$$\mathbf{F}_{centrifugalMO} = -\frac{\hbar^2}{m_e a^2 b^2} D \mathbf{i}_\xi .$$

184. The system of claim 183 wherein force balance equation for the σ-MO of the carbon monoxide molecule is

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 a b^2} D + \frac{\hbar^2}{2 m_e a^2 b^2} D - \left(1 + \left(\frac{1}{Z_1} + \frac{1}{Z_2}\right)\right) \frac{\hbar^2}{2 m_e a^2 b^2} D$$

$$a=\left(2+\frac{1}{Z_1}+\frac{1}{Z_2}\right)a_0$$

185. The system of claim 184 wherein the Coulombic force is

$$\mathbf{F}_{Coulomb}=\frac{e^2}{8\pi\varepsilon_0 ab^2}D\mathbf{i}_\xi;$$

the spin pairing force is

$$\mathbf{F}_{spin-pairing}=\frac{\hbar^2}{2m_e a^2 b^2}D\mathbf{i}_\xi$$

the force on the electrons of the MO due to two paired electrons in at least one shell with $n_e=2$ is

$$\mathbf{F}_{diamagneticMO1}=-\frac{\hbar^2}{2m_e a^2 b^2}D\mathbf{i}_\xi;$$

the force $\mathbf{F}_{diamagneticMO2}$ of the nitric oxide radical comprising nitrogen with charge $Z_1=7$ and $|L_1|=\hbar$ and $|L_2|=\sqrt{\frac{3}{4}}\hbar$ and oxygen with $Z_2=8$ and $|L_3|=\hbar$ given by the corresponding sum of the contributions is

$$\mathbf{F}_{diamagneticMO2}=-\left(\frac{1}{Z_1}+\frac{\sqrt{\frac{3}{4}}}{Z_1}+\frac{1}{Z_2}\right)\frac{\hbar^2}{2m_e a^2 b^2}D\mathbf{i}_\xi, \text{ and}$$

the centrifugal force is

$$\mathbf{F}_{centrifugalMO}=-\frac{\hbar^2}{m_e a^2 b^2}D\mathbf{i}_\xi.$$

186. The system of claim 185 wherein the general force balance equation for the σ-MO of the nitric oxide radical is the same as that of CN:

$$\frac{\hbar^2}{m_e a^2 b^2}D=\frac{e^2}{8\pi\varepsilon_0 ab^2}D+\frac{\hbar^2}{2m_e a^2 b^2}D-\left(1+\frac{1}{Z_1}+\frac{\sqrt{\frac{3}{4}}}{Z_1}+\frac{1}{Z_2}\right)\frac{\hbar^2}{2m_e a^2 b^2}D$$

$$a=\left(2+\frac{1}{Z_1}+\frac{\sqrt{\frac{3}{4}}}{Z_1}+\frac{1}{Z_2}\right)a_0$$

where $Z_1=7$ and $Z_2=8$ for NO and $Z_1=6$ and $Z_2=7$ for CN.

187. The system of claims 186 and 63 wherein the distance from the origin of the H_2-type-ellipsoidal-MO to each focus c', the internuclear distance $2c'$, and the length of the semiminor axis of the prolate spheroidal H_2-type MO $b=c$ are solved from the semimajor axis a.

188. The system of claim 187 wherein the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e=n_1c_1c_2\frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}};$$

The potential energy of the two nuclei is

$$V_p=n_1\frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}};$$

The kinetic energy of the electrons is

$$T=n_1c_1c_2\frac{\hbar^2}{2m_ea\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}},\text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m=n_1c_1c_2\frac{-\hbar^2}{4m_ea\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}},\text{ and}$$

the total energy, E_T, is given by the sum of the energy terms plus $E(AO)$:

$$E_T=V_e+T+V_m+V_p$$

$$E_T=-\frac{n_1e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]$$

$$=-\frac{n_1e^2}{8\pi\varepsilon_0c'}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital to which the MO is energy matched.

189. The system of claim 188 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib}$, and

the total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}.$$

190. The system of claim 189 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

the total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{ -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2 \left(2 - \frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'} - 1\right]\left[1 + \sqrt{\frac{2\hbar\sqrt{\frac{c_1 c_2 e^2}{4\pi\varepsilon_o a^3}}}{m_e c^2}}\right] - n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

where R is b or a, n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital to which the MO is energy matched.

191. The system of claim 190 wherein the bond comprises a H_2-type MO with four paired electron wherein the formation of the H_2-type MO by the contribution of two electrons from each participating atom results in a diamagnetic force between the remaining atomic electrons and the H_2-type MO which causes the H_2-type MO to move to greater principal axes than would result with the Coulombic force alone.

192. The system of claim 191 wherein the integer increase of the central field and the resulting increased Coulombic as well as magnetic central forces on the remaining atomic electrons of each atom decrease the radius of the corresponding shell such that the energy minimum is achieved that is lower than that of the reactant atoms.

193. The system of claim 192 wherein the general equation for the central Coulomb force on the outer-most shell (nth where $n = Z - 2$) electron due to the nucleus and the inner electrons is given by:

$$\mathbf{F}_{ele} = \frac{3e^2}{4\pi\varepsilon_0 r_n^2}\mathbf{i}_r$$

for $r > r_{n-1}$.

194. The system of claim 193 wherein the general equation for $\mathbf{F}_{diamagnetic}$ due to the p-orbital contribution is given by

$$\mathbf{F}_{diamagnetic} = -A\frac{\hbar^2}{12m_e r_n^2 r_3}\sqrt{\frac{3}{4}}\mathbf{i}_r$$

195. The system of claim 194 wherein the general equation for $\mathbf{F}_{mag\ 2}$ is given by

$$\mathbf{F}_{mag\ 2} = B\frac{1}{Z}\frac{\hbar^2}{m_e r_n^2 r_3}\sqrt{s(s+1)}\mathbf{i}_r$$

196. The system of claim 195 wherein the general equation for $\mathbf{F}_{diamagnetic\ 2}$ due to the binding of the p-orbital electron having an electric field of +2 outside of its radius is given by

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{2}{3}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{m_e r_n^4}10\sqrt{s(s+1)}\mathbf{i}_r$$

197. The system of claim 196 wherein the general equation for $\mathbf{F}_{mag\ 3}$, due to the contribution of a $2p$ electron from each binding atom in the formation of the σ MO that gives rise to a paramagnetic force on the remaining two $2p$ electrons that pair, is given by

$$\mathbf{F}_{mag\ 3} = C\frac{\hbar^2}{4m_e r_n^3}\sqrt{s(s+1)}\mathbf{i}_r$$

198. The system of claim 197 wherein the parameters A, B, and C are zero or a positive integer such that the resulting energy of the molecule is minimized and the electron angular momentum is conserved in the formation of the specie.

199. The system of claim 198 wherein the radius of the $2p$ shell is calculated by equating the outward centrifugal force to the sum of the electric and diamagnetic and paramagnetic forces:

$$\frac{m_e v_n^2}{r_n} = \left(\begin{array}{l}\frac{3e^2}{4\pi\varepsilon_0 r_n^2} - A\frac{\hbar^2}{12m_e r_n^2 r_3}\sqrt{s(s+1)} + B\frac{\hbar^2}{Zm_e r_n^2 r_3}\sqrt{s(s+1)} \\ -\left[\frac{2}{3}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{r_n^4 m_e}10\sqrt{s(s+1)} + C\frac{\hbar^2}{4m_e r_n^3}\sqrt{s(s+1)}\end{array}\right) \quad (13.626)$$

200. The system of claim 199 wherein the radius of the $2p$ shell is calculated by equating the outward centrifugal force to the sum of the electric and diamagnetic and paramagnetic forces where the velocity given by $v_n = \frac{\hbar}{m_e r_n}$ and $s = \frac{1}{2}$ gives:

$$\frac{\hbar^2}{m_e r_n^3} - C\frac{\hbar^2}{4m_e r_n^3}\sqrt{\frac{3}{4}} = \frac{3e^2}{4\pi\varepsilon_0 r_n^2} - A\frac{\hbar^2}{12m_e r_n^2 r_3}\sqrt{\frac{3}{4}} + B\frac{\hbar^2}{Zm_e r_6^2 r_3}\sqrt{\frac{3}{4}} - \left[\frac{2}{3}\right]\left(1-\frac{\sqrt{2}}{2}\right)\frac{r_3\hbar^2}{r_n^4 m_e}10\sqrt{\frac{3}{4}}$$

201. The system of claim 200 wherein the general equation for the radius of the shell of the remaining electrons is given by

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$$r_6 = \frac{\dfrac{a_0\left(1-C\frac{\sqrt{3}}{8}\right)}{\left(3-\left(\frac{A}{12}-\frac{B}{Z}\right)\frac{\sqrt{3}}{2r_3}\right)} \pm a_0\sqrt{\left(\dfrac{1-C\frac{\sqrt{3}}{8}}{\left(3-\left(\frac{A}{12}-\frac{B}{Z}\right)\frac{\sqrt{3}}{2r_3}\right)}\right)^2 + \dfrac{20\sqrt{3}\left(\left[\frac{2}{3}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_3\right)}{\left(3-\left(\frac{A}{12}-\frac{B}{Z}\right)\frac{\sqrt{3}}{2r_3}\right)}}}{2}$$

r_3 *in units of* a_0

202. The system of claim 201 wherein the radii r_3 are given by

$$r_4 = r_3 = \frac{\left(\dfrac{a_0\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)} \pm a_o\sqrt{\dfrac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^2}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)^2} + 4\dfrac{\left[\frac{Z-3}{Z-2}\right]r_1 10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_1}\right)}}\right)}{2}$$

r_1 *in units of* a_o

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203. The system of claim 202, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^{n-4}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by:

$$r_1 = r_2 = a_o \left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right];$$

and two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by:

$$r_4 = r_3 = \frac{\left(\frac{a_0 \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)} \pm a_o \sqrt{\frac{\left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)^2}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)^2} + 4 \frac{\left[\frac{Z-3}{Z-2} \right] r_1 10 \sqrt{\frac{3}{4}}}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)}} \right)}{2}$$

r_1 in units of a_o

204. The system of claim 203 wherein the force balance of a double-bond MO corresponds to that of a second pair of two electrons binding to a molecular ion having $+2e$ at each focus and a first bound pair such that the forces are the same as those of a molecule ion having $+e$ at each focus.

205. The system of claim 204 wherein the forces on the electrons of the MO are the Coulombic force:

$$\mathbf{F}_{Coulomb} = \frac{e^2}{8\pi\varepsilon_0 ab^2} D\mathbf{i}_\xi;$$

the spin pairing force:

$$\mathbf{F}_{spin-pairing} = \frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi ;$$

the diamagnetic force:

$$\mathbf{F}_{diamagneticMO1} = -\frac{n_e \hbar^2}{4m_e a^2 b^2} D\mathbf{i}_\xi$$

where n_e is the total number of electrons that interact with the binding σ-MO electron;

the force on the pairing electron of the σ MO:

$$\mathbf{F}_{diamagneticMO2} = -\frac{1}{Z}\frac{|L|\hbar}{2m_e a^2 b^2} D\mathbf{i}_\xi$$

where $|L|$ is the magnitude of the angular momentum of each atom at a focus that is the source of the diamagnetism at the σ-MO, and

the centrifugal force:

$$\mathbf{F}_{centrifugalMO} = -\frac{\hbar^2}{m_e a^2 b^2} D\mathbf{i}_\xi , \text{ and}$$

the force balance of the centrifugal force equated to the Coulombic and magnetic forces is solved for the length of the semimajor axis.

206. The system of claim 205 wherein the forces on the electrons of the NO_2 MO are the Coulombic force:

$$\mathbf{F}_{Coulomb} = \frac{e^2}{8\pi\varepsilon_0 ab^2} D\mathbf{i}_\xi ;$$

the spin pairing force:

$$\mathbf{F}_{spin-pairing} = \frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi ;$$

the diamagnetic force $\mathbf{F}_{diamagneticMO1}$ for each σ-MO of the NO_2 molecule due to the two paired electrons in the $O2p$ shell with $n_e = 2$:

$$\mathbf{F}_{diamagneticMO1} = \frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi$$

which is also the corresponding force of NO;

$\mathbf{F}_{diamagneticMO2}$ of the nitrogen dioxide molecule comprising nitrogen with charge $Z_1 = 7$

and $|L_1| = \hbar$ and $|L_2| = \sqrt{\frac{3}{4}}\hbar$ and the two oxygen atoms, each with $Z_2 = 8$ and $|L_3| = \hbar$ given by the corresponding sum of the contributions:

$$\mathbf{F}_{diamagneticMO2} = \left(\frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{2}{Z_2} \right) \frac{\hbar^2}{2m_e a^2 b^2} D\mathbf{i}_\xi$$

which is also the corresponding force of NO and CN except the term due to oxygen is twice that of NO due to the two oxygen atoms of NO_2, and

the centrifugal force

$\mathbf{F}_{centrifugalMO} = -\frac{\hbar^2}{m_e a^2 b^2} D\mathbf{i}_\xi$, and

the force balance of the centrifugal force equated to the Coulombic and magnetic forces is solved for the length of the semimajor axis.

207. The system of claim 206 wherein the force balance equation for the σ-MOs of NO_2 with $Z_1 = 7$ and $Z_2 = 8$ is

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\varepsilon_0 ab^2} D + \frac{\hbar^2}{2m_e a^2 b^2} D - \left(1 + \frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{2}{Z_2} \right) \frac{\hbar^2}{2m_e a^2 b^2} D$$

$$a = \left(2 + \frac{1}{Z_1} + \frac{\sqrt{\frac{3}{4}}}{Z_1} + \frac{2}{Z_2} \right) a_0$$

208. The system of claims 207 and 63 wherein the distance from the origin of the H_2-type-ellipsoidal-MO to each focus c', the internuclear distance $2c'$, and the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ are solved from the semimajor axis a.

209. The system of claim 208 wherein the sum $E_T(molecule, AOs)$ of the Coulombic energy change of the AO electrons of the participating atoms or ions of the bonds of the specie is the sum of the contributions over all such atoms or ions given by using the initial radius r_n of the atom or ion and the final radius r_{n-2} of the binding shell of the atom or ion and by considering that the central Coulombic field decreases by an integer for each successive electron of the shell:

$$E_T(molecule, AOs) = \sum_{m=n_1-4}^{n_1-3} \frac{(Z-m)e^2}{8\pi\varepsilon_0}\left(\frac{1}{r_{n_1-2}} - \frac{1}{r_{n_1}}\right)$$

where the subscript designates the exemplary atom 1 of the bond.

210. The system of claim 209 wherein the sum $E_T(molecule, AOs)$ of the Coulombic energy change of the AO electron of a participating atom of a bond wherein all of the electrons of the shell of the AO are contributed to the bond is given by the sum of the corresponding ionization energies of the AO electrons.

211. The system of claim 210 wherein energy of the double bond MO is match to the participating AOs and the potential energy of the four electrons in the central field of the nuclei at the foci is

$$V_e = 2^2 n_1 c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}};$$

The potential energy of the two nuclei is

$$V_p = 2^2 n_1 \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}};$$

The kinetic energy of the electrons is

$$T = 2n_1 c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = 2^2 n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms plus $E(AO)$:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -\frac{2^2 n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1c_2(2)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]+n_1E(AO)$$

$$=-\frac{2^2 n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1c_2(2)\ln\frac{a+c'}{a-c'}-1\right]+n_1E(AO)$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital to which the MO is energy matched.

212. The system of claim 211 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib}$, and

the total energy is

$$E_T = V_e + T + V_m + V_p + E(AO) + \overline{E}_{osc}.$$

213. The system of claim 212 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$E_T = -2^2\frac{n_1e^2}{8\pi\varepsilon_0c'}\left[c_1c_2(2)\ln\frac{a+c'}{a-c'}-1\right]+n_1E(AO)+\overline{E}_{osc}$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond, and $E(AO)$ is the energy of the at least one atomic orbital to which the MO is energy matched.

214. The system of claim 213 wherein the energy components of are V_e, V_p, T, V_m, and E_T, except that the terms based on charge are multiplied by four and the kinetic energy term is multiplied by two due to each σ-MO double bond.

215. The system of claim 214 wherein the potential energy of the four electrons of double bond in the central field of the nuclei at the foci is

$$V_e = 2^2 n_1 c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}};$$

The potential energy of the two nuclei is

$$V_p = 2^2 n_1 \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}};$$

The kinetic energy of the electrons is

$$T = 2n_1 c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = 2^2 n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}} \ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -\frac{2^2 n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1 c_2 (2)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} - 1\right].$$

$$= -\frac{2^2 n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2 (2)\ln\frac{a+c'}{a-c'} - 1\right]$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

216. The system of claim 215 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib}, \text{ and}$$

the total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}.$$

217. The system of claim 216 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$E_T = -\frac{2^2 n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2 (2)\ln\frac{a+c'}{a-c'} - 1\right] + \overline{E}_{osc}$$

n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

218. The system of claim 217 wherein the total energy of the specie is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms, the change in the energy of the AOs or HOs upon forming the bond, the change in magnetic energy with bond formation, and the energy of oscillation in the transition state.

219. The system of claim 218 wherein the total energy of the specie is the sum over all of the component groups wherein the total energy of each said group is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms, the change in the energy of the AOs or HOs upon forming the bond, the change in magnetic energy with bond formation, and the energy of oscillation in the transition state.

220. The system of claim 219 wherein the change in magnetic energy is given by

$$E(magnetic) = \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_n^3} = \frac{8\pi\mu_o\mu_B^2}{r_n^3}$$

where r_n^3 is the radius of the atom that reacts to form the bond.

221. The system of claim 220 wherein the bond energy of the molecular or molecular ion is difference in the energy of the total energy of the starting species and the total energy of the specie.

222. The system of claim 221 wherein the bond energy of a specific bond of the molecular or molecular ion is difference in the energy of the sum of the energies of the atoms and any change in energy of any groups formed with the starting atoms and the total energy of the bond of the specie.

223. The system of claim 222 wherein the total energy of a molecule, $E_T(molecule)$, is given by the sum of:

the sum of the energies of the electrons donated to each bond,

the sum of the energies of electrons of at least one other atom donated to the bonds,

the sum over the participating atoms of each AO contribution due to the decrease in radius with the formation of each bond, and

the σ MO energy contribution per bond.

224. The system of claim 223 wherein the total energy of a molecule, $E_T(molecule)$, is given by the sum of:

the sum of the energies of the electrons donated to each bond such that all of the electrons of the shell are donated,

the sum of the energies of electrons of at least one other atom donated to the bonds,

the sum over the participating atoms of each AO contribution due to the decrease in radius with the formation of each bond, and

the σ MO energy contribution per bond.

225. The system of claim 223 wherein the total energy of CO_2, $E_T(CO_2)$, is given by the sum of $E(ionization;\ C)$ and $E(ionization;\ C^+)$, the sum of the energies of the first and second electrons of carbon donated to each double bond, the sum of $E(ionization;\ O)$ and two times $E(ionization;\ O^+)$, the energies of the first and second electrons of oxygen donated to the double bonds, two times $E_T(O,2p)$, the $O2p$ AO contribution due to the decrease in radius with the formation of each bond and two times $E_T(C=O,\sigma)$, the σ MO contribution:

$$E_T(CO_2)=\begin{pmatrix}E(ionization;\ C)+E(ionization;\ C^+)+E(ionization;\ O)\\+2E(ionization;\ O^+)+2E_T(O,2p)+2E_T(C=O,\sigma)\end{pmatrix}$$

$$=\begin{pmatrix}11.26030\ eV+24.38332\ eV+13.61806\ eV\\+2(35.11730\ eV)+2(-32.12759\ eV)\\-2\left(\dfrac{4e^2}{8\pi\varepsilon_0\sqrt{\dfrac{2aa_0}{3}}}\left(\left(\dfrac{3}{2}\right)\ln\dfrac{a+\sqrt{\dfrac{2aa_0}{3}}}{a-\sqrt{\dfrac{2aa_0}{3}}}-1\right)\right)\end{pmatrix}$$

$$=\begin{pmatrix}11.26030\ eV+24.38332\ eV+13.61806\ eV\\+2(35.11730\ eV)+2(-32.12759\ eV)-2(55.25423\ eV)\end{pmatrix}$$

$$=-55.26841\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

226. The system of claim 225 wherein the total energy of a molecule, $E_{T+osc}(molecule)$ is given by the sum of $E_T(molecule)$ and $\overline{E}_{osc}$.

227. The system of claim 226 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_{hv}\sqrt{\frac{2\overline{E}_K}{m_e c^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right), \text{ and}$$

where the angular frequency of the reentrant oscillation in the transition state is

$$\omega = \sqrt{\frac{c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}}{m_e}};$$

the kinetic energy, E_K, is given by Planck's:

$$\overline{E}_K = \hbar\omega = \hbar\sqrt{\frac{c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}}{m_e}};$$

the Doppler energy of the electrons of the reentrant orbit is

$$\overline{E}_D \cong E_{hv}\sqrt{\frac{2\overline{E}_K}{m_e c^2}} = E_{hv}\sqrt{\frac{2\hbar\sqrt{\frac{c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}}{m_e}}}{m_e c^2}}$$

$\overline{E}_{osc}$ is given by the sum of and $\overline{E}_{Kvib}$, the vibrational energy:

$$\overline{E}_{osc}(molecule) = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_{hv}\sqrt{\frac{2\hbar\sqrt{\frac{c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}}{m_e}}}{m_e c^2}} + E_{vib}\right)$$

where R is b or a, n_1 is the number of equivalent bonds of the MO, c_{BO} is the bond-order factor which is 1 for a single bond, 4 for a double bond, and 9 for a triplet bond, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

228. The system of claim 227 wherein E_{hv} is given by $E_T(molecule)/2$ in the case of a double bond such that

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = E_T(molecule)/2\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}.$$

229. The system of claim 228 wherein E_{hv} of a molecule having n_1 bonds is given by $E_T(molecule)/n_1$ such that

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_T(molecule)/n_1\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right).$$

230. The system of claim 229 wherein E_{hv} of a molecule having n_1 bonds is given by $E_T(H_2)$ such that

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_T(H_2)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right).$$

where $E_T(H_2) = -31.63537\ eV$ is the total energy of the hydrogen molecule, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

231. The system of claim 230 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_{hv}\sqrt{\frac{2\overline{E}_K}{m_e c^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right), \text{ and}$$

where the angular frequency of the reentrant oscillation in the transition state is determined by the force between the central field and the electrons in the transition state; said force and its derivative are given by

$$f(R) = -c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}$$

and

$$f'(a) = 2c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}$$

such that the angular frequency of the oscillation is given by

$$\omega = \sqrt{\frac{\left[\frac{-3}{a} f(a) - f'(a)\right]}{m_e}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO} \frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}}{m_e}}$$

where R is b or a, c_{BO} is the bond-order factor which is 1 for a single bond, 4 for a double bond, and 9 for a triplet bond, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

232. The system of claim 231 wherein the nucleus of the B atom and the nucleus of the A atom comprise the foci of each H_2-type ellipsoidal MO of the $A-B$ bond and the parameters of the point of intersection of each H_2-type ellipsoidal MO and the A-atom AO are determined from the polar equation of the ellipse:

$$r = r_0 \frac{1+e}{1+e\cos\theta'}$$

233. The system of claim 232 wherein the radius of the A shell is r_A, and the polar radial coordinate of the ellipse and the radius of the A shell are equal at the point of intersection such that

$$r_A = (a-c') \frac{1+\frac{c'}{a}}{1+\frac{c'}{a}\cos\theta'}, \text{ and}$$

the polar angle θ' at the intersection point is given by

$$\theta' = \cos^{-1}\left(\frac{a}{c'}\left((a-c')\frac{1+\frac{c'}{a}}{a_0} - 1\right)\right)$$

234. The system of claim 233 wherein the angle $\theta_{A\,AO}$ the radial vector of the A AO makes with the internuclear axis is

$$\theta_{A\,AO} = 180° - \theta'$$

235. The system of claim 234 wherein the distance from the point of intersection of the orbitals to the internuclear axis must be the same for both component orbitals such that the angle $\omega t = \theta_{H_2MO}$ between the internuclear axis and the point of intersection of each H_2-type ellipsoidal MO with the A radial vector obeys the following relationship:

$$r_A \sin\theta_{A\,AO} = b \sin\theta_{H_2MO}$$

such that

$$\theta_{H_2MO} = \sin^{-1} \frac{r_a \sin\theta_{A\,AO}}{b};$$

the distance d_{H_2MO} along the internuclear axis from the origin of H_2-type ellipsoidal MO to the point of intersection of the orbitals is given by

$d_{H_2MO} = a\cos\theta_{H_2MO}$, and

the distance $d_{A\,AO}$ along the internuclear axis from the origin of the A atom to the point of intersection of the orbitals is given by

$$d_{A\,AO} = c' - d_{H_2MO}.$$

236. The system of claim 235 where the bond angle is determined from the zero energy condition of the total energy of the potential bond between any pair of terminal atoms.

237. The system of claim 236 where the force constant k' of a H_2-type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{c_1 c_2 2e^2}{4\pi\varepsilon_o}$$

where c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie and c_2 is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the chemical bond.

238. The system of claim 237 where the distance from the origin of the MO to each focus c' is given by:

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2k' a}} = \sqrt{\frac{aa_0}{2k'}};$$

the internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2k'}};$$

the length of the semiminor axis of the prolate spheroidal MO $b = c$ is given by

$b = \sqrt{a^2 - c'^2}$, and

and, the eccentricity, e, is

$$e = \frac{c'}{a}.$$

239. The system of claim 238 wherein the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e = c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}};$$

The potential energy of the two nuclei is

$$V_p = \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2 - b^2}};$$

The kinetic energy of the electrons is

$$T = c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}}, \text{ and}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}}, \text{ and}$$

The total energy, E_T, is given by the sum of the energy terms:

$$E_T = V_e + T + V_m + V_p$$

$$E_T = -\frac{e^2}{8\pi\varepsilon_o\sqrt{a^2 - b^2}}\left[c_1 c_2\left(2 - \frac{a_0}{a}\right)\ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1\right].$$

$$= -\frac{e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2 - \frac{a_0}{a}\right)\ln\frac{a + c'}{a - c'} - 1\right]$$

where c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

240. The system of claim 239 wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib} = \left(V_e + T + V_m + V_p\right)\sqrt{\frac{2\overline{E}_K}{Mc^2}} + n_1 \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}, \text{ and}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \overline{E}_{osc}$$

$$E_T = -\left\{\frac{e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2 - \frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'} - 1\right]\left[1 + \sqrt{\frac{2\hbar\sqrt{\frac{c_1 c_2 e^2}{4\pi\varepsilon_o a^3}}{m_e}}{m_e c^2}}\right] - \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right\}$$

where c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

241. The system of claim 240 wherein the vibrational energy $\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}$ is given by

$$+\frac{1}{2}\hbar\sqrt{\frac{\frac{c_1 e^2}{8\pi\varepsilon_o a^3} - \frac{e^2}{8\pi\varepsilon_o\left(a+c'\right)^3}}{\mu}}$$

where μ is the reduced mass of the nuclei.

242. The system of claim 241 wherein the energy components of are V_e, V_p, T, V_m, and E_T, except that the terms based on charge are multiplied by four and the kinetic energy term is multiplied by two due to a σ-MO double bond.

243. The system of claim 242 wherein $c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2k' a}} = \sqrt{\frac{aa_0}{2k'}}$ is substituted into the equation for E_T which is set equal to zero, and the semimajor axis is solved.

244. The system of claims 243 and 63 wherein the distance from the origin of the H_2-type-ellipsoidal-MO to each focus c', the internuclear distance $2c'$, and the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ are solved from the semimajor axis a.

245. The system of claim 244 wherein with $2c'_{A-B}$ defined as the internuclear distance of each $A-B$ bond and $C = 2c'_{B-B}$ defined as the internuclear distance of the two terminal B atoms, the bond angle between the $A-B$ bonds is given by the law of cosines is

$$\theta = \cos^{-1}\left(\frac{2\left(2c'_{A-B}\right)^2 - \left(2c'_{B-B}\right)^2}{2\left(2c'_{A-B}\right)^2}\right)$$

246. The system of claim 245 wherein the specie comprises more than two bonds with one $A-B$ bound along an axis defined as the vertical or z-axis and any two $A-B$ bonds form an isosceles triangle; the angle of the bonds from the defined axis is determined from the geometrical relationships:

the distance $d_{origin-B}$ from the origin to the nucleus of a terminal B atom is given by

$$d_{origin-B} = \frac{2c'_{B-B}}{2\sin 60°};$$

the height along the z-axis from the origin to A nucleus d_{height} is given by

$$d_{height} = \sqrt{\left(2c'_{A-B}\right)^2 - \left(d_{origin-B}\right)^2}\,, \text{ and}$$

the angle θ_v of each $A-B$ bond from the z-axis is given by

$$\theta_v = \tan^{-1}\left(\frac{d_{origin-B}}{d_{height}}\right).$$

247. The system of claim 246 wherein the vibrational energies are determined by the forces between the central field and the electrons and those between the nuclei; said electron-central-field force and its derivative are given by

$$f(R) = -c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3}$$

and

$$f'(a) = 2c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3};$$

said nuclear repulsion force and its derivative are given by

$$f(2c') = \frac{e^2}{8\pi\varepsilon_0 (2c')^2}$$

and

$$f'(2c') = -\frac{e^2}{4\pi\varepsilon_0 (2c')^3}$$

such that the angular frequency of the oscillation is given by

$$\omega = \sqrt{\frac{\left[\frac{-3}{a}f(a) - f'(a)\right]}{\mu}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO}\frac{c_1 c_2 e^2}{4\pi\varepsilon_0 R^3} - \frac{e^2}{8\pi\varepsilon_0 (2c')^2}}{\mu}}$$

where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass of the nuclei, R is b or a, c_{BO} is the bond-order factor which is 1 for a single bond, 4 for a double bond, and 9 for a triplet bond, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie, and c_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of each chemical bond.

248. The system of claim 247 wherein the transition-state vibrational energy, $E_{vib}(0)$, given by Planck's equation is:

$$E_{vib}(0) = \hbar\omega$$

249. The system of claim 248 wherein the energy $\tilde{\nu}_\upsilon$ of state υ is given by

$$\tilde{\nu}_\upsilon = \upsilon\omega_0 - \upsilon(\upsilon - 1)\omega_0 x_0, \quad \upsilon = 0,1,2,3...$$

where

$$\omega_0 x_0 = \frac{hc\omega_0^2}{4D_0}$$

ω_0 is the frequency of the $\upsilon = 1 \rightarrow \upsilon = 0$ transition, and D_0 is the bond dissociation energy.

250. The system of claim 249 wherein ω_0 is given by

$$\omega_0 = E_{vib}(0) - 2\omega_0 x_0, \text{ and}$$

$$\omega_0 = E_{vib}(0) - 2\frac{hc\omega_0^2}{4D_0}$$

such that

$$\omega_0^2 + \frac{2D_0}{hc}\omega_0 - \frac{2D_0}{hc}E_{vib}(0) = 0, \text{ and}$$

$$\omega_0 = \frac{-\frac{2D_0}{hc} \pm \sqrt{\left(\frac{2D_0}{hc}\right)^2 + 4\frac{2D_0}{hc}E_{vib}(0)}}{2}.$$

251. The system of claim 250 wherein B_e, the rotational parameter, for $A-B$ is given by:

$$B_e = \frac{\hbar^2}{2I_e hc}$$

where $I = \mu r^2$, $r = 2c'$, and μ is the reduced mass.

252. The system of claim 251 wherein the vibrational energy levels of the $A-A$ and $A-B$ bonds of the specie are solved as sets of coupled atomic harmonic oscillators wherein each atom of a chain of bonds is further coupled to at least one additional harmonic oscillators by using the Lagrangian, the differential equation of motion, and the eigenvalue solutions wherein the spring constants are derived from the central forces.

253. The system of claim 252 wherein the vibrational energy levels of the $C-C$ bonds of C_nH_{2n+2} are solved as $n-1$ sets of coupled carbon harmonic oscillators wherein each carbon is further coupled to two or three equivalent H harmonic oscillators by using the Lagrangian, the differential equation of motion, and the eigenvalue solutions wherein the spring constants are derived from the central forces.

254. The system of claim 253 wherein $E_D(C_nH_{2n+2})$, the total bond dissociation energy of C_nH_{2n+2}, is given as the sum of the energy components due to the two methyl groups, $n-2$ methylene groups, and $n-1$ $C-C$ bonds.

255. The system of claim 254 wherein the total bond dissociation energy of C_nH_{2n+2} is given by

$$E_D(C_nH_{2n+2}) = E_D(C-C)_{n-1} + 2E_{D_{alkane}}\left({}^{12}CH_3\right) + (n-2)E_{D_{alkane}}\left({}^{12}CH_2\right)$$
$$= (n-1)(4.32754\ eV) + 2(12.49186\ eV) + (n-2)(7.83016\ eV)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

256. The system of claim 255 wherein the exact solution for the dimensional parameters, charge density functions, and energies of molecules are determined using the results for the determination of C_nH_{2n+2} and the functional groups as basis sets that are linearly combined.

257. The system of claim 256 wherein one or more of the hydrogen atoms of the solution for C_nH_{2n+2} are substituted with one or more of the previously solved functional groups or derivative functional groups to give the parameters of a desired molecule.

258. The system of claim 257 wherein the parameters of a given molecule are given by energy matching each group to C_nH_{2n+2}.

259. The system of claim 258 wherein substitution of one or more H's of C_nH_{2n+2} with functional groups from the list of CH_3, other C_nH_{2n+2} groups, $H_2C=CH_2$, $HC\equiv CH$, F, Cl, O, OH, NH, NH_2, CN, NO, NO_2, CO, CO_2, and C_6H_6 give the solutions of branched alkanes, alkenes, and alkynes, alkyl halides, ethers, alcohols, amides, amines, nitriles, alkyl nitrosos, alkyl nitrates, aldehydes, ketones, carboxylic acids, esters, and substituted aromatics.

260. A composition of matter comprising a plurality of atoms, the improvement comprising a novel property or use discovered by calculation of at least one of
a bond distance between two of the atoms,
a bond angle between three of the atoms, and
a bond energy between two of the atoms,
orbital intercept distances and angles,

charge-density functions of atomic, hybridized, and molecular orbitals,
the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.

261. A composition of matter according to claim 260, wherein the novel property is a new pharmaceutical use.

262. A composition of matter according to claim 261 that is novel, wherein the novel property is stability at room temperature of a new arrangement of atoms or ions.

263. A novel composition of matter discovered by calculating at least one of
a bond distance between two of the atoms,
a bond angle between three of the atoms, and
a bond energy between two of the atoms,
orbital intercept distances and angles,
charge-density functions of atomic, hybridized, and molecular orbitals,
the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.

264. A system of determining at least one of
a bond distance between two of the atoms,
a bond angle between three of the atoms, and
a bond energy between two of the atoms,
orbital intercept distances and angles,
charge-density functions of atomic, hybridized, and molecular orbitals,
wherein the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration.

265. The system of claim 264, further comprising discovering a new composition of matter.

266. The system of claim 1, wherein the nature of said specie includes the nature of a chemical bond thereof.

267. The system of claim 1, wherein at least one bond angle between three atoms is computed and displayed.

268. The system of claim 1, wherein at least one bond distance between two atoms is computed and displayed.

269. The system of claim 1, wherein at least one geometric component is computed and displayed.

270. The system of claim 1, wherein at least one potential energy between an electron and a nucleus is computed.

271. The system of claim 1, wherein at least one potential energy between two nuclei is computed.

272. The system of claim 1, wherein at least one kinetic energy of an electron is computed.

273. The system of claim 1, wherein at least one magnetic energy between electrons is computed.

274. The system of claim 1, wherein at least one total energy of a bond is computed.

275. The system of claim 1, wherein at least one change in atomic energy between atoms due to bonding is computed.

276. The system of claim 1, further comprising at least one database of functional groups and at least one database of molecules, molecular ions, and/or molecular radicals, characterized in that the functional groups, molecules, molecular ions, and molecular radicals having the nature of their chemical bonds computed by the Maxwillian solutions of charge, mass, and current density, or both databases being combined into one database or split into multiple databases, and the processing means being in communication with the databases or combined database.

277. The system of claim 1, further comprising at least one database of functional groups having the nature of their chemical bonds computed by the Maxwillian solutions of charge, mass, and current density.

278. The system of claim 276, further comprising means for selecting a desired first functional group, characterized in that the selected functional group is displayed with open bonds being displayed, means for selecting an open bond, means for selecting a second functional group to be bound to the first functional group, characterized in that the second functional group is displayed with open bonds being displayed, means for selecting an open bond on the second functional group, and means for combining the selected bonds, whereby at least a portion of a desired molecule is displayed.

279. The system of claim 276, further comprising selecting and combining functional groups until a desired molecule is displayed.

280. The system of claim 277, further comprising means for selecting a desired first functional group, characterized in that the selected functional group is displayed with open bonds being displayed, means for selecting an open bond, means for selecting a second functional group to be bound to the first functional group, characterized in that the second functional group is displayed with open bonds being displayed, means for selecting an open bond on the second functional group, and means for combining the selected bonds, whereby at least a portion of a desired molecule is displayed.

281. The system of claim 277, further comprising selecting and combining functional groups until a desired molecule is displayed.

282. The system of claim 1, further comprising a means for inputting the chemical structure of a desired molecule and parsing the inputted molecule into functional groups.

283. The system of claim 282, further comprising a database of functional groups having the nature of their chemical bonds computed by the Maxwillian solutions of charge, mass, and current density, characterized in that the processing means combines the functional groups and the desired molecule is displayed.

284. The system of claim 282, wherein the chemical structure is imputed using a Simplified Molecular Input Line Entry System.

285. The system of claim 283, wherein the chemical structure is imputed using a Simplified Molecular Input Line Entry System.

286. The system of claim 282, wherein the Simplified Molecular Input Line Entry System is SMILES.

287. The system of claim 283, wherein the Simplified Molecular Input Line Entry System is SMILES.

288. The system according to claim 1, wherein the force generalized constant k' of a H_2-type ellipsoidal MO due to the equivalent of two point charges at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\varepsilon_0} \qquad (15.1)$$

where C_1 is the fraction of the H_2-type ellipsoidal molecular orbital basis function of a chemical bond of the specie and C_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of the chemical bond.

289. The system according to claim 1, wherein the distance from the origin of the MO to each focus c' is given by:

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2C_1C_2 a}} = \sqrt{\frac{aa_0}{2C_1C_2}} \tag{15.2}$$

the internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2C_1C_2}} \tag{15.3}$$

the length of the semiminor axis of the prolate spheroidal MO $b = c$ is given by

$$b = \sqrt{a^2 - c'^2} \tag{15.4}$$

and, the eccentricity, e, is

$$e = \frac{c'}{a} \tag{15.5}.$$

290. The system according to claim 289, wherein a potential energy of the electrons in the central field of the nuclei at the foci is

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \tag{15.6}$$

where n_1 is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by c_{BO}, the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

291. The system according to claim 1, wherein the potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2 - b^2}} \tag{15.7}.$$

292. The system according to claim 1, wherein the kinetic energy of the electrons is

$$T = n_1 c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} \tag{15.8}$$

where n_1 is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by c_{BO}, the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

293. The system according to claim 1, wherein the energy, V_m, of the magnetic force between the electrons is

$$V_m = n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} \tag{15.9}$$

where n_1 is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by c_{BO}, the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

294. The system according to claim 1, wherein total energy of the H_2-type prolate spheroidal MO, $E_T(_{H_2MO})$, is given by the sum of the energy terms:

$$E_T(_{H_2MO}) = V_e + T + V_m + V_p \tag{15.10}$$

$$\begin{aligned} E_T(_{H_2MO}) &= -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right] \\ &= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right] \end{aligned} \tag{15.11}$$

where n_1 is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by c_{BO}, the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

295. The system according to claim 1, wherein the total energy $E_T\left(atom, msp^3\right)$ (m is the integer of the valence shell) of the AO electrons and the hybridized shell is given by the sum of energies of successive ions of the atom over the n electrons comprising total electrons of the at least one AO shell according to the formula:

$$E_T\left(atom, msp^3\right) = -\sum_{m=1}^{n} IP_m \qquad (15.12$$

where IP_m is the m th ionization energy (positive) of the atom.

296. The system according to claim 295, wherein the radius r_{msp^3} of the hybridized shell is given by:

$$r_{msp^3} = \sum_{q=Z-n}^{Z-1} \frac{-(Z-q)e^2}{8\pi\varepsilon_0 E_T\left(atom, msp^3\right)} \qquad (15.13).$$

297. The system according to claim 295, wherein the Coulombic energy $E_{Coulomb}\left(atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by

$$E_{Coulomb}\left(atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} \qquad (15.14).$$

298. The system of claim 296, wherein in the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r of the AO electron:

$$E(magnetic) = \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r^3} = \frac{8\pi\mu_o\mu_B^2}{r^3} \qquad (15.15)$$

then, the energy $E\left(atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(atom, msp^3\right)$ and $E(magnetic)$:

$$E\left(atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r^3} \qquad (15.16).$$

299. The system according to claim 295, wherein the total energy $E_T\left(mol.atom, msp^3\right)$ (m is the integer of the valence shell) of the HO electrons is given by the sum of energies of successive ions of the atom over the n electrons comprising total electrons of the at least one initial AO shell and the hybridization energy:

$$E_T\left(mol.atom, msp^3\right) = E\left(atom, msp^3\right) - \sum_{m=2}^{n} IP_m \tag{15.17}$$

where IP_m is the m th ionization energy (positive) of the atom and the sum of $-IP_1$ plus the hybridization energy is $E\left(atom, msp^3\right)$.

300. The system of claim 299, wherein the radius r_{msp^3} of the hybridized shell is given by:

$$r_{msp^3} = \left(\sum_{q=Z-n}^{Z-1} (Z-q) - s(0.25) \right) \frac{-e^2}{8\pi\varepsilon_0 E_T\left(mol.atom, msp^3\right)} \tag{15.18}$$

where $s = 1, 2, 3$ for a single, double, and triple bond, respectively.

301. The system of claim 299, wherein the Coulombic energy $E_{Coulomb}\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by

$$E_{Coulomb}\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} \tag{15.19}.$$

302. The system of claim 298, wherein in the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r of the AO electron given by Eq. (15.15). Then, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$:

$$E\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \tag{15.20}$$

$E_T\left(atom-atom,msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of the atom-atom-bond MO is given by the difference between $E\left(mol.atom,msp^3\right)$ and $E\left(atom,msp^3\right)$:

$$E_T\left(atom-atom,msp^3\right)=E\left(mol.atom,msp^3\right)-E\left(atom,msp^3\right) \quad (15.21).$$

303. The system of claim 295, wherein $E_{Coulomb}\left(mol.atom,msp^3\right)$ is one of:

$E_{Coulomb}\left(C_{ethylene},2sp^3\right)$, $E_{Coulomb}\left(C_{ethane},2sp^3\right)$, $E_{Coulomb}\left(C_{acetylene},2sp^3\right)$, and $E_{Coulomb}\left(C_{alkane},2sp^3\right)$;

$E_{Coulomb}\left(atom,msp^3\right)$ is one of $E_{Coulomb}\left(C,2sp^3\right)$ and $E_{Coulomb}\left(Cl,3sp^3\right)$;

$E\left(mol.atom,msp^3\right)$ is one of $E\left(C_{ethylene},2sp^3\right)$, $E\left(C_{ethane},2sp^3\right)$, $E\left(C_{acetylene},2sp^3\right)$ $E\left(C_{alkane},2sp^3\right)$;

$E\left(atom,msp^3\right)$ is one of and $E\left(C,2sp^3\right)$ and $E\left(Cl,3sp^3\right)$;

$E_T\left(atom-atom,msp^3\right)$ is one of $E\left(C-C,2sp^3\right)$, $E\left(C=C,2sp^3\right)$, and. $E\left(C\equiv C,2sp^3\right)$;

atom msp^3 is one of $C2sp^3$, $Cl3sp^3$

$E_T\left(atom-atom\left(s_1\right),msp^3\right)$ is $E_T\left(C-C,2sp^3\right)$ and $E_T\left(atom-atom\left(s_2\right),msp^3\right)$ is $E_T\left(C=C,2sp^3\right)$, and

r_{msp^3} is one of r_{C2sp^3}, $r_{ethane2sp^3}$, $r_{ethylene2sp^3}$, $r_{acetylene2sp^3}$, $r_{alkane2sp^3}$, and r_{Cl3sp^3}.

In the case of the $C2sp^3$ HO, the initial parameters (Eqs. (14.142-14.146)) are

$$r_{2sp^3}=\sum_{n=2}^{5}\frac{(Z-n)e^2}{8\pi\varepsilon_0\left(e148.25751\ eV\right)}=\frac{10e^2}{8\pi\varepsilon_0\left(e148.25751\ eV\right)}=0.91771a_0 \quad (15.22)$$

$$E_{Coulomb}\left(C,2sp^3\right)=\frac{-e^2}{8\pi\varepsilon_0 r_{2sp^3}}=\frac{-e^2}{8\pi\varepsilon_0 0.91771a_0}=-14.82575\ eV \quad (15.23)$$

$$E(magnetic)=\frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_3\right)^3}=\frac{8\pi\mu_o\mu_B^2}{\left(0.84317a_0\right)^3}=0.19086\ eV \quad (15.24)$$

$$E\left(C,2sp^3\right)=\frac{-e^2}{8\pi\varepsilon_0 r_{2sp^3}}+\frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(r_3\right)^3}$$
$$=-14.82575\ eV+0.19086\ eV \quad (15.25)$$
$$=-14.63489\ eV$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

304. The system of claim 300, wherein

$$\sum_{q=Z-n}^{Z-1}(Z-q)=10 \quad (15.26)$$

Equations (14.147) and (15.17) give

$$E_T\left(mol.atom,msp^3\right)=E_T\left(C_{ethane},2sp^3\right)=-151.61569\ eV \quad (15.27)$$

and using Eqs. (15.18-15.28), the final values of r_{C2sp^3}, $E_{Coulomb}\left(C2sp^3\right)$, and $E\left(C2sp^3\right)$, and the resulting $E_T\left(C\overset{BO}{-}C,C2sp^3\right)$ of the MO due to charge donation from the HO to the MO

where $C\overset{BO}{-}C$ refers to the bond order of the carbon-carbon bond for different values of the parameter s are given in Table 15.1.

Table 15.1:

MO Bond Order (BO)	s 1	s 2	$r_{C2sp^3}(a_0)$ Final	$E_{Coulomb}\left(C2sp^3\right)$(eV) Final	$E\left(C2sp^3\right)$ (eV) Final	$E_T\left(C\overset{BO}{-}C,C2sp^3\right)$ (eV)
I	1	0	0.87495	-15.55033	-15.35946	-0.72457
II	2	0	0.85252	-15.95955	-15.76868	-1.13379
III	3	0	0.83008	-16.39089	-16.20002	-1.56513
IV	4	0	0.80765	-16.84619	-16.65532	-2.02043

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

305. The system of claim 295, wherein a minimum-energy bond with the constraint that it must meet the energy matching condition for all MOs at all HOs or AOs, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell of each bonding atom is the average of $E\left(mol.atom, msp^3\right)$ for two different values of s:

$$E\left(mol.atom, msp^3\right) = \frac{E\left(mol.atom\left(s_1\right), msp^3\right) + E\left(mol.atom\left(s_2\right), msp^3\right)}{2} \qquad (15.28).$$

306. The system of claim 305, wherein in the case, $E_T\left(atom - atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of each atom-atom-bond MO, is average for two different values of s:

$$E_T\left(atom - atom, msp^3\right) = \frac{E_T\left(atom - atom\left(s_1\right), msp^3\right) + E_T\left(atom - atom\left(s_2\right), msp^3\right)}{2} \qquad (15.29).$$

307. The system of claim 305, wherein a first MO and its HOs comprising a linear combination of bond orders and a second MO that shares a HO with the first. In addition to the mutual HO, the second MO comprises another AO or HO having a single bond order or a mixed bond order, in order for the two MOs to be energy matched, the bond order of the second MO and its HOs or its HO and AO is a linear combination of the terms corresponding to the bond order of the mutual HO and the bond order of the independent HO or AO, and in general, $E_T\left(atom - atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of each atom-atom-bond MO, is a weighted linear sum for different values of s that matches the energy of the bonded MOs, HOs, and AOs:

$$E_T\left(atom - atom, msp^3\right) = \sum_{n=1}^{N} c_{s_n} E_T\left(atom - atom\left(s_n\right), msp^3\right) \qquad (15.30)$$

where c_{s_n} is the multiple of the BO of s_n. The radius r_{msp^3} of the *atom* msp^3 shell of each bonding atom is given by the Coulombic energy using the initial energy $E_{Coulomb}\left(atom, msp^3\right)$ and $E_T\left(atom - atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of each atom-atom-bond MO:

$$r_{msp^3} = \frac{-e^2}{8\pi\varepsilon_0 a_0 \left(E_{Coulomb}\left(atom, msp^3\right) + E_T\left(atom - atom, msp^3\right)\right)} \tag{15.31}$$

where $E_{Coulomb}\left(C2sp^3\right) = -14.825751\ eV$.

308. The system of claim 307, wherein the Coulombic energy $E_{Coulomb}\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by Eq. (15.19).

309. The system of claim 308, wherein in the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ (Eq. (15.15)) at the initial radius r of the AO electron. Then, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$ (Eq. (15.20)).

310. The system of claim 308, wherein, $E_T\left(atom - atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of the atom-atom-bond MO is given by the difference between $E\left(mol.atom, msp^3\right)$ and $E\left(atom, msp^3\right)$ given by Eq. (15.21).

311. The system of claim 310, wherein using the equation (15.23) for $E_{Coulomb}\left(C, 2sp^3\right)$ in equation (15.31), the single bond order energies given by Eqs. (15.18-15.27) and shown in Table 15.1, and the linear combination energies (Eqs. (15.28-15.30)), the parameters of linear combinations of bond orders and linear combinations of mixed bond orders are given in Table 15.2, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

312. The system of claim 295, wherein the radius r_{mol2sp^3} of the $C2sp^3$ HO of a carbon atom of a given specie is calculated using Eq. (14.514) by considering

$\sum E_{T_{mol}}\left(MO,2sp^3\right)$, the total energy donation to each bond with which it participates in bonding.

313. The system of claim 1, wherein equation for the radius is given by

$$r_{mol2sp^3}=\frac{-e^2}{8\pi\varepsilon_0\left(E_{Coulomb}\left(C,2sp^3\right)+\sum E_{T_{mol}}\left(MO,2sp^3\right)\right)}=\frac{e^2}{8\pi\varepsilon_0\left(e14.825751\ eV+\sum\left|E_{T_{mol}}\left(MO,2sp^3\right)\right|\right)} \quad (15.32).$$

314. The system of 295, wherein the Coulombic energy $E_{Coulomb}\left(mol.atom,msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by Eq. (15.19).

315. The system of claim 295, in the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ (Eq. (15.15)) at the initial radius r of the AO electron. Then, the energy $E\left(mol.atom,msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(mol.atom,msp^3\right)$ and $E(magnetic)$ (Eq. (15.20)).

316. The system of claim 315, wherein for the $C2sp^3$ HO of each methyl group of an alkane contributes $-0.92918\ eV$ (Eq. (14.513)) to the corresponding single $C-C$ bond; the corresponding $C2sp^3$ HO radius is given by Eq. (14.514). The $C2sp^3$ HO of each methylene group of C_nH_{2n+2} contributes $-0.92918\ eV$ to each of the two corresponding $C-C$ bond MOs, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

317. The system of claim 316, wherein the radius (Eq. (15.32)), the Coulombic energy (Eq. (15.19)), and the energy (Eq. (15.20)) of each alkane methylene group are

$$r_{alkaneC_{methylene}2sp^3} = \frac{-e^2}{8\pi\varepsilon_0\left(E_{Coulomb}\left(C,2sp^3\right)+\sum E_{T_{alkane}}\left(methylene\ C-C,2sp^3\right)\right)}$$
$$= \frac{e^2}{8\pi\varepsilon_0\left(e14.825751\ eV+e0.92918\ eV+e0.92918\ eV\right)}$$
$$= 0.81549a_0$$

(15.33)

$$E_{Coulomb}\left(C_{methylene}2sp^3\right) = \frac{-e^2}{8\pi\varepsilon_0\left(0.81549a_0\right)} = -16.68412\ eV \quad (15.34)$$

$$E\left(C_{methylene}2sp^3\right) = \frac{-e^2}{8\pi\varepsilon_0\left(0.81549a_0\right)} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(0.84317a_0\right)^3} = -16.49325\ eV \quad (15.35)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

318. The system of claim 316, wherein in the determination of the parameters of functional groups, heteroatoms bonding to $C2sp^3$ HOs to form MOs are energy matched to the $C2sp^3$ HOs, the radius and the energy parameters of a bonding heteroatom are given by the same equations as those for $C2sp^3$ HOs.

319. The system of claim 318, wherein using Eqs. (15.15), (15.19-15.20), (15.24), and (15.32) in a generalized fashion, the final values of the radius of the HO or AO, $r_{Atom.HO.AO}$, $E_{Coulomb}\left(mol.atom,msp^3\right)$, and $E\left(C_{mol}2sp^3\right)$ are calculated using $\sum E_{T_{group}}\left(MO,2sp^3\right)$, the total energy donation to each bond with which an atom participates in bonding corresponding to the values of $E_T\left(C\overset{BO}{-}C,C2sp^3\right)$ of the MO due to charge donation from the AO or HO to the MO given in Tables 15.1 and 15.2 and the final values of $r_{Atom.HO.AO}$, $E_{Coulomb}\left(mol.atom,msp^3\right)$, and $E\left(C_{mol}2sp^3\right)$ calculated using the values of $E_T\left(C\overset{BO}{-}C,C2sp^3\right)$ given in Tables 15.1 and 15.2 are shown in Tables 15.3A and 15.3B in the specification, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

320. The system of claim 319, wherein the energy of the MO is matched to each of the participating outermost atomic or hybridized orbitals of the bonding atoms wherein the energy match includes the energy contribution due to the AO or HO's donation of charge to the MO.

321. The system of claim 320, wherein the force constant k' (Eq. (15.1)) is used to determine the ellipsoidal parameter c' (Eq. (15.2)) of the each H_2-type-ellipsoidal-MO in terms of the central force of the foci, c' is substituted into the energy equation (from Eq. (15.11))) which is set equal to n_1 times the total energy of H_2 where n_1 is the number of equivalent bonds of the MO and the energy of H_2, $-31.63536831\ eV$, Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

322. The system of claim 321, wherein the energy equation and the relationship between the axes, the dimensions of the MO are solved, the energy equation has the semimajor axis a as it only parameter, the solution of the semimajor axis a allows for the solution of the other axes of each prolate spheroid and eccentricity of each MO (Eqs. (15.3-15.5)), and the parameter solutions then allow for the component and total energies of the MO to be determined.

323. The system of claim 1, wherein the total energy, $E_T(_{H_2MO})$, is given by the sum of the energy terms (Eqs. (15.6-15.11)) plus $E_T(AO/HO)$:

$$E_T(_{H_2MO}) = V_e + T + V_m + V_p + E_T(AO/HO) \quad (15.36)$$

$$E_T(_{H_2MO}) = -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]+E_T(AO/HO)$$

$$=-\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]+E_T(AO/HO) \quad (15.37)$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type

ellipsoidal MO basis function of a chemical bond of the group, c_2 is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of each chemical bond, and $E_T(AO/HO)$ is the total energy comprising the difference of the energy $E(AO/HO)$ of at least one atomic or hybrid orbital to which the MO is energy matched and any energy component $\Delta E_{H_2MO}(AO/HO)$ due to the AO or HO's charge donation to the MO.

324. The system of claim 323, wherein

$$E_T(AO/HO) = E(AO/HO) - \Delta E_{H_2MO}(AO/HO) \quad (15.38)$$

325. The system of claim 324, wherein as specific examples, $E_T(AO/HO)$ is one from the group of

$E_T(AO/HO) = E(O2p\ shell) = -E(ionization;\ O) = -13.6181\ eV$;

$E_T(AO/HO) = E(N2p\ shell) = -E(ionization;\ N) = -14.53414\ eV$;

$E_T(AO/HO) = E(C, 2sp^3) = -14.63489\ eV$;

$E_T(AO/HO) = E_{Coulomb}(Cl, 3sp^3) = -14.60295\ eV$;

$E_T(AO/HO) = E(ionization;\ C) + E(ionization;\ C^+)$;

$E_T(AO/HO) = E(C_{ethane}, 2sp^3) = -15.35946\ eV$;

$E_T(AO/HO) = +E(C_{ethylene}, 2sp^3) - E(C_{ethylene}, 2sp^3)$;

$E_T(AO/HO) = E(C, 2sp^3) - 2E_T(C=C, 2sp^3) = -14.63489\ eV - (-2.26758\ eV)$;

$E_T(AO/HO) = E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) = 16.20002\ eV$;

$E_T(AO/HO) = E(C, 2sp^3) - 2E_T(C \equiv C, 2sp^3) = -14.63489\ eV - (-3.13026\ eV)$;

$E_T(AO/HO) = E(C_{benzene}, 2sp^3) - E(C_{benzene}, 2sp^3)$;

$E_T(AO/HO) = E(C, 2sp^3) - E_T(C=C, 2sp^3) = -14.63489\ eV - (-1.13379\ eV)$, and

$E_T(AO/HO) = E(C_{alkane}, 2sp^3) = -15.56407\ eV$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

326. The system of claim 1, wherein to solve the bond parameters and energies, $c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2C_1C_2 a}} = \sqrt{\frac{aa_0}{2C_1C_2}}$ (Eq. (15.2)) is substituted into $E_T(H_2MO)$ to give

$$E_T(H_2MO) = -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right]+E_T(AO/HO)$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]+E_T(AO/HO)$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0\sqrt{\frac{aa_0}{2C_1C_2}}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2C_1C_2}}}{a-\sqrt{\frac{aa_0}{2C_1C_2}}}-1\right]+E_T(AO/HO)$$

(15.39)

wherein the total energy is set equal to $E(basis\ energies)$ which in the most general case is given by the sum of a first integer n_1 times the total energy of H_2 minus a second integer n_2 times the total energy of H, minus a third integer n_3 times the valence energy of $E(AO)$ (e.g. $E(N) = -14.53414\ eV$) where the first integer can be 1,2,3..., and each of the second and third integers can be 0,1,2,3....

327. The system of claim 326, wherein

$$E(basis\ energies) = n_1(-31.63536831\ eV) - n_2(-13.605804\ eV) - n_3E(AO)$$

(15.40)

in the case that the MO bonds two atoms other than hydrogen, $E(basis\ energies)$ is n_1 times the total energy of H_2 where n_1 is the number of equivalent bonds of the MO and the energy of H_2, $-31.63536831\ eV$, Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO:

$$E(basis\ energies) = n_1(-31.63536831\ eV) \quad (15.41)$$

$E_T(H_2MO)$, is set equal to $E(basis\ energies)$, and the semimajor axis a is solved.

328. The system of claims 289 or 326, wherein the semimajor axis a is solved from the equation of the form:

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$$-\frac{n_1 e^2}{8\pi\varepsilon_0\sqrt{\frac{aa_0}{2C_1C_2}}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2C_1C_2}}}{a-\sqrt{\frac{aa_0}{2C_1C_2}}}-1\right]+E_T\left(AO/HO\right)=E(basis\ energies) \quad (15.42)$$

The distance from the origin of the H_2-type-ellipsoidal-MO to each focus c', the internuclear distance $2c'$, and the length of the semiminor axis of the prolate spheroidal H_2-type MO $b=c$ are solved from the semimajor axis a using Eqs. (15.2-15.4).

329. The system of claim 328, wherein the component energies are given by Eqs. (15.6-15.9) and (15.39).

330. The system of claim 323, wherein the total energy of the MO of the functional group, $E_T(MO)$, is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms and $E_T\left(atom-atom, msp^3.AO\right)$, the change in the energy of the AOs or HOs upon forming the bond.

331. The system of claim 330, wherein from Eqs. (15.39-15.40), $E_T(MO)$ is

$$E_T(MO)=E(basis\ energies)+E_T\left(atom-atom, msp^3.AO\right) \quad (15.43)$$

332. The system of claim 331, wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\overline{E}_{osc}$ is the sum of the Doppler, $\overline{E}_D$, and average vibrational kinetic energies, $\overline{E}_{Kvib}$:

$$\overline{E}_{osc}=n_1\left(\overline{E}_D+\overline{E}_{Kvib}\right)=n_1\left(E_{h\nu}\sqrt{\frac{2\overline{E}_K}{m_ec^2}}+\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right) \quad (15.44)$$

where n_1 is the number of equivalent bonds of the MO, k is the spring constant of the equivalent harmonic oscillator, and μ is the reduced mass.

333. The system of claim 332, wherein the angular frequency of the reentrant oscillation in the transition state corresponding to $\overline{E}_D$ is determined by the force between the central

field and the electrons in the transition state.

334. The system of claim 333,wherein the force and its derivative are given by

$$f(R) = -c_{BO}\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3} \qquad (15.45)$$

and

$$f'(a) = 2c_{BO}\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3} \qquad (15.46)$$

such that the angular frequency of the oscillation in the transition state is given by

$$\omega = \sqrt{\frac{\left[\frac{-3}{a}f(a) - f'(a)\right]}{m_e}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO}\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}} \qquad (15.47)$$

where R is the semimajor axis a or the semiminor axis b depending on the eccentricity of the bond that is most representative of the oscillation in the transition state, c_{BO} is the bond-order factor which is 1 for a single bond and when the MO comprises n_1 equivalent single bonds as in the case of functional groups, c_{BO} is 4 for an independent double bond as in the case of the CO_2 and NO_2 molecules and 9 for an independent triplet bond, C_{1o} is the fraction of the H_2-type ellipsoidal MO basis function of the oscillatory transition state of a chemical bond of the group, and C_{2o} is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the transition state of the chemical bond. Typically, $C_{1o} = C_1$ and $C_{2o} = C_2$, the kinetic energy, E_K, corresponding to $\overline{E}_D$ is given by Planck's equation for functional groups:

$$\overline{E}_K = \hbar\omega = \hbar\sqrt{\frac{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}} \qquad (15.48)$$

335. The system of claim 334, wherein the Doppler energy of the electrons of the reentrant orbit is

$$\overline{E}_D \cong E_{h\nu}\sqrt{\frac{2\overline{E}_K}{m_e c^2}} = E_{h\nu}\sqrt{\frac{2\hbar\sqrt{\frac{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}}}{m_e c^2}} \qquad (15.49)$$

$\overline{E}_{osc}$ given by the sum of $\overline{E}_D$ and $\overline{E}_{Kvib}$ is

$$\overline{E}_{osc}(group) = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_{hv}\sqrt{\frac{2\hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}}{m_e c^2}} + E_{vib}\right) \quad (15.50)$$

E_{hv} of a group having n_1 bonds is given by $E_T(MO)/n_1$ such that

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_T(MO)/n_1\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right) \quad (15.51)$$

$E_{T+osc}(Group)$ is given by the sum of $E_T(MO)$ (Eq. (15.42)) and $\overline{E}_{osc}$ (Eq. (15.51)):

$$E_{T+osc}(Group) = E_T(MO) + \overline{E}_{osc}$$

$$= \left(\left(\begin{array}{l} -\frac{n_1 e^2}{8\pi\varepsilon_0\sqrt{\frac{aa_0}{2C_1C_2}}}\left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2C_1C_2}}}{a-\sqrt{\frac{aa_0}{2C_1C_2}}} - 1\right] \\ +E_T\left(AO/HO\right) + E_T\left(atom-atom, msp^3.AO\right) \end{array}\right)\right.$$

$$\left.\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}{m_e}}{m_e c^2}}\right] + n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right)$$

$$= \left(E(basis\ energies) + E_T\left(atom-atom, msp^3.AO\right)\right)\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}{m_e}}{m_e c^2}}\right] + n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}$$

(15.52).

336. The system of claim 335, wherein the total energy of the functional group $E_T(group)$ is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms, $E(basis\ energies)$, the change in the energy of the AOs or HOs upon forming the bond ($E_T\left(atom-atom, msp^3.AO\right)$), the energy of

oscillation in the transition state, and the change in magnetic energy with bond formation, E_{mag}.

337. The system of claim 336, wherein from Eq. (15.52), the total energy of the group $E_T(Group)$ is

$$E_T(Group) = \left(\begin{array}{l} \left(E(basis\ energies) + E_T\left(atom - atom, msp^3.AO\right) \right) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}}{m_e c^2}} \right] \\ + n_1 \overline{E}_{Kvib} + E_{mag} \end{array} \right) \quad (15.53).$$

338. The system of claim 337, wherein the change in magnetic energy E_{mag} which arises due to the formation of unpaired electrons in the corresponding fragments relative to the bonded group is given by

$$E_{mag} = c_3 \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} = c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} \qquad (15.54)$$

where r^3 is the radius of the atom that reacts to form the bond and c_3 is the number of electron pairs.

$$E_T(Group) = \left(\begin{array}{l} \left(E(basis\ energies) + E_T\left(atom - atom, msp^3.AO\right) \right) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}}{m_e c^2}} \right] \\ + n_1 \overline{E}_{Kvib} + c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} \end{array} \right) \quad (15.55).$$

339. The system of claim 338, wherein the total bond energy of the group $E_D(Group)$ is the negative difference of the total energy of the group (Eq. (15.55)) and the total energy of the starting species given by the sum of $c_4 E_{initial}\left(c_4\ AO/HO\right)$ and $c_5 E_{initial}\left(c_5\ AO/HO\right)$:

$$E_{D\,(Group)} = -\left(\begin{array}{l} \left(E(basis\ energies) + E_T\left(atom - atom, msp^3.AO\right)\right)\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}}{m_e c^2}}\right] \\ +n_1\overline{E}_{Kvib} + c_3\frac{8\pi\mu_o\mu_B^2}{r_n^3} - \left(c_4 E_{initial}\left(AO/HO\right) + c_5 E_{initial}\left(c_5\ AO/HO\right)\right) \end{array} \right)$$

(15.56).

340. The system of claim 336, wherein in the case of organic molecules, the atoms of the functional groups are energy matched to the $C2sp^3$ HO such that

$$E\left(AO/HO\right) = -14.63489\ eV \qquad (15.57)$$

For examples of E_{mag} from previous sections:

$$E_{mag}\left(C2sp^3\right) = c_3\frac{8\pi\mu_o\mu_B^2}{r^3} = c_3\frac{8\pi\mu_o\mu_B^2}{\left(0.91771a_0\right)^3} = c_3 0.14803\ eV \qquad (15.58)$$

$$E_{mag}\left(O2p\right) = c_3\frac{8\pi\mu_o\mu_B^2}{r^3} = c_3\frac{8\pi\mu_o\mu_B^2}{a_0^3} = c_3 0.11441\ eV \qquad (15.59)$$

$$E_{mag}\left(N2p\right) = c_3\frac{8\pi\mu_o\mu_B^2}{r^3} = c_3\frac{8\pi\mu_o\mu_B^2}{\left(0.93084a_0\right)^3} = c_3 0.14185\ eV \quad (15.60).$$

341. The system of claim 340, wherein in the general case of the solution of an organic functional group, the geometric bond parameters are solved from the semimajor axis and the relationships between the parameters by first using Eq. (15.42) to arrive at a, the remaining parameters are determined using Eqs. (15.1-15.5), the energies are given by Eqs. (15.52-15.59), and to meet the equipotential condition for the union of the H_2-type-ellipsoidal-MO and the HO or AO of the atom of a functional group, the factor c_2 of a H_2-type ellipsoidal MO in principal Eqs. (15.42) and (15.52) may given by

(i) one:

$$c_2 = 1 \quad (15.61)$$

(ii) the ratio that is less than one of $13.605804\ eV$, the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), and the magnitude of the

Coulombic energy of the participating AO or HO of the atom, $E_{Coulomb}\left(MO.atom, msp^3\right)$ given by Eqs. (15.19) and (15.31-15.32). For $\left|E_{Coulomb}\left(MO.atom, msp^3\right)\right|$>13.605804 eV :

$$c_2 = \frac{\frac{e^2}{8\pi\varepsilon_0 a_0}}{\frac{e^2}{8\pi\varepsilon_0 r_{A-B\ AorBsp^3}}} = \frac{13.605804\ eV}{\left|E_{Coulomb}\left(MO.atom, msp^3\right)\right|} \quad (15.62)$$

For $\left|E_{Coulomb}\left(MO.atom, msp^3\right)\right|$<13.605804 eV :

$$c_2 = \frac{\frac{e^2}{8\pi\varepsilon_0 r_{A-B\ AorBsp^3}}}{\frac{e^2}{8\pi\varepsilon_0 a_0}} = \frac{\left|E_{Coulomb}\left(MO.atom, msp^3\right)\right|}{13.605804\ eV} \quad (15.63)$$

(iii) the ratio that is less than one of 13.605804 eV , the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), and the magnitude of the valence energy, $E(valence)$, of the participating AO or HO of the atom where $E(valence)$ is the ionization energy or $E\left(MO.atom, msp^3\right)$ given by Eqs. (15.20) and (15.31-15.32). For $|E(valence)|$>13.605804 eV :

$$c_2 = \frac{\frac{e^2}{8\pi\varepsilon_0 a_0}}{\frac{e^2}{8\pi\varepsilon_0 r_{A-B\ AorBsp^3}}} = \frac{13.605804\ eV}{|E(valence)|} \quad (15.64)$$

For $|E(valence)|$<13.605804 eV :

$$c_2 = \frac{\frac{e^2}{8\pi\varepsilon_0 r_{A-B\ AorBsp^3}}}{\frac{e^2}{8\pi\varepsilon_0 a_0}} = \frac{|E(valence)|}{13.605804\ eV} \quad (15.65)$$

(iv) the ratio that is less than one of the magnitude of the Coulombic energy of the participating AO or HO of a first atom, $E_{Coulomb}\left(MO.atom, msp^3\right)$ given by Eqs. (15.19) and (15.31-15.32), and the magnitude of the valence energy, $E(valence)$, of the participating AO or HO of a second atom to which the first is energy matched where $E(valence)$ is the

ionization energy or $E\left(MO.atom,msp^3\right)$ given by Eqs. (15.20) and (15.31-15.32). For $\left|E_{Coulomb}\left(MO.atom,msp^3\right)\right| > E(valence)$:

$$c_2 = \frac{|E(valence)|}{\left|E_{Coulomb}\left(MO.atom,msp^3\right)\right|} \qquad (15.66)$$

For $\left|E_{Coulomb}\left(MO.atom,msp^3\right)\right| < E(valence)$:

$$c_2 = \frac{\left|E_{Coulomb}\left(MO.atom,msp^3\right)\right|}{|E(valence)|} \qquad (15.67)$$

(v) the ratio that is less than one of the magnitude of the valence-level energies, $E_n(valence)$, of the AO or HO of the nth participating atom of two that are energy matched where $E(valence)$ is the ionization energy or $E\left(MO.atom,msp^3\right)$ given by Eqs. (15.20) and (15.31-15.32):

$$c_2 = \frac{E_1(valence)}{E_2(valence)} \qquad (15.68)$$

(vi) the factor that is the ratio of the hybridization factor $c_2(1)$ of the valence AO or HO of a first atom and the hybridization factor $c_2(2)$ of the valence AO or HO of a second atom to which the first is energy matched where $c_2(n)$ is given by Eqs. (15.62-15.68); alternatively c_2 is the hybridization factor $c_2(1)$ of the valence AOs or HOs a first pair of atoms and the hybridization factor $c_2(2)$ of the valence AO or HO a third atom or second pair to which the first two are energy matched:

$$c_2 = \frac{c_2(1)}{c_2(2)} \qquad (15.69)$$

(vii) the factor that is the product of the hybridization factor $c_2(1)$ of the valence AO or HO of a first atom and the hybridization factor $c_2(2)$ of the valence AO or HO of a second atom to which the first is energy matched where $c_2(n)$ is given by Eqs. (15.62-15.69); alternatively c_2 is the hybridization factor $c_2(1)$ of the valence AOs or HOs a first pair of

atoms and the hybridization factor $c_2(2)$ of the valence AO or HO a third atom or second pair to which the first two are energy matched:

$$c_2 = c_2(1)c_2(2) \qquad (15.70)$$

The hybridization factor c_2 corresponds to the force constant k (Eqs. (11.65) and (13.58)). In the case that the valence or Coulombic energy of the AO or HO is less than 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), then C_2 corresponding to k' (Eq. (15.1)) is given by Eqs. (15.62-15.70).

342. The system of claim 341, wherein specific examples of the factors c_2 and C_2 of a H_2-type ellipsoidal MO of Eq. (15.51) given in following sections are

$$c_2(C2sp^3HO\ to\ F) = \frac{E(C,2sp^3)}{E(F)} c_2(C2sp^3HO) = \frac{-14.63489\ eV}{-17.42282\ eV}(0.91771) = 0.77087;$$

$$C_2(C2sp^3HO\ to\ Cl) = \frac{E(Cl)}{E(C,2sp^3)} c_2(C2sp^3HO) = \frac{-12.96764\ eV}{-14.63489\ eV}(0.91771) = 0.81317;$$

$$C_2(C2sp^3HO\ to\ Br) = \frac{E(Br)}{E(C,2sp^3)} c_2(C2sp^3HO) = \frac{-11.81381\ eV}{-14.63489\ eV}(0.91771) = 0.74081;$$

$$C_2(C2sp^3HO\ to\ I) = \frac{E(I)}{E(C,2sp^3)} c_2(C2sp^3HO) = \frac{-10.45126\ eV}{-14.63489\ eV}(0.91771) = 0.65537;$$

$$c_2(C2sp^3HO\ to\ O) = \frac{E(O)}{E(C,2sp^3)} c_2(C2sp^3HO) = \frac{-13.61806\ eV}{-14.63489\ eV}(0.91771) = 0.85395;$$

$$c_2(H\ to\ 1°N) = \frac{E(N)}{E(C,2sp^3)} = \frac{-14.53414\ eV}{-15.35946\ eV} = 0.94627;$$

$$c_2(C2sp^3HO\ to\ N) = \frac{E(N)}{E(C,2sp^3)} c_2(C2sp^3HO) = \frac{-14.53414\ eV}{-14.63489\ eV}(0.91771) = 0.91140;$$

$$c_2(H\ to\ 2°N) = \frac{E(N)}{E(C,2sp^3)} = \frac{-14.53414\ eV}{-15.56407\ eV} = 0.93383;$$

$$C_2(S3p\ to\ H) = \frac{E(S,3p)}{E(H)} = \frac{-10.36001\ eV}{-13.60580\ eV} = 0.76144;$$

$$C_2(C2sp^3HO\ to\ \mathrm{S}) = \frac{E(S)}{E(C,2sp^3)} c_2(C2sp^3HO) = \frac{-10.36001\ eV}{-14.63489\ eV}(0.91771) = 0.64965;$$

$$c_2\left(O\ to\ S3sp^3\ to\ C2sp^3HO\right)=\frac{E(O)}{E(S)}c_2\left(C2sp^3HO\right)$$
$$=\frac{-13.61806\ eV}{-10.36001\ eV}(0.91771);$$
$$=1.20632$$

$$c_2\left(S3sp^3\right)=\frac{E_{Coulomb}\left(S3sp^3\right)}{E(H)}=\frac{-11.57099\ eV}{-13.60580\ eV}=0.85045;$$

$$C_2\left(C2sp^3HO\ to\ S3sp^3\right)=\frac{E\left(S3sp^3\right)}{E\left(C,2sp^3\right)}c_2\left(S3sp^3\right)=\frac{-11.52126\ eV}{-14.63489\ eV}(0.85045)=0.66951;$$

$$C_2\left(S3sp^3\ to\ O\ to\ C2sp^3HO\right)=\frac{E\left(S,3sp^3\right)}{E(O,2p)}c_2\left(C2sp^3HO\right)$$
$$=\frac{-11.52126\ eV}{-13.61806\ eV}(0.91771)\ ;$$
$$=0.77641$$

$$c_2\left(O\ to\ N2p\ to\ C2sp^3HO\right)=\frac{E(O)}{E(N)}c_2\left(C2sp^3HO\right)$$
$$=\frac{-13.61806\ eV}{-14.53414\ eV}(0.91771);$$
$$=0.85987$$

$$c_2\left(N2p\ to\ O2p\right)=\frac{c_2\left(C2sp^3HO\ to\ N\right)}{c_2\left(C2sp^3HO\ to\ O\right)}=\frac{0.91140}{0.85395}=1.06727;$$

$$C_2\left(benzeneC2sp^3HO\right)=c_2\left(benzeneC2sp^3HO\right)=\frac{13.605804\ eV}{15.95955\ eV}=0.85252;$$

$$c_2\left(arylC2sp^3HO\ to\ O\right)=\frac{E(O)}{E\left(C,2sp^3\right)}c_2\left(arylC2sp^3HO\right)$$
$$=\frac{-13.61806\ eV}{-14.63489\ eV}(0.85252)\qquad;$$
$$=0.79329$$

$$c_2\left(H\ to\ \text{anline}\ N\right)=\frac{E(N)}{E\left(C,2sp^3\right)}=\frac{-14.53414\ eV}{-15.76868\ eV}=0.92171,$$

$$c_2\left(arylC2sp^3HO\ to\ N\right)=\frac{E(N)}{E\left(C,2sp^3\right)}c_2\left(arylC2sp^3HO\right)$$
$$=\frac{-14.53414\ eV}{-14.63489\ eV}(0.85252)$$
$$=0.84665$$

$$c_2\left(H\ to\ \text{anline}\ N\right)=\frac{E(N)}{E\left(C,2sp^3\right)}=\frac{-14.53414\ eV}{-15.76868\ eV}=0.92171;$$

$$c_2\left(arylC2sp^3HO\ to\ N\right)=\frac{E(N)}{E\left(C,2sp^3\right)}c_2\left(arylC2sp^3HO\right)$$

$$=\frac{-14.53414\ eV}{-14.63489\ eV}(0.85252) \quad , \quad \text{and}$$

$$=0.84665$$

$$C_2\left(S3p\ to\ \text{aryl-type}\ C2sp^3HO\right)=\frac{E\left(S,3p\right)}{E\left(C,2sp^3\right)}=\frac{-10.36001\ eV}{-15.76868\ eV}=0.65700.$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

343. The system of claim 1, wherein the parameters of the point of intersection of each H_2-type ellipsoidal MO and the A-atom AO are determined from the polar equation of the ellipse:

$$r=r_0\frac{1+e}{1+e\cos\theta'} \qquad (15.71).$$

344. The system of claim 343, wherein the radius of the A shell is r_A, and the polar radial coordinate of the ellipse and the radius of the A shell are equal at the point of intersection such that

$$r_A=(a-c')\frac{1+\frac{c'}{a}}{1+\frac{c'}{a}\cos\theta'} \qquad (15.72).$$

345. The system of claim 344, wherein the polar angle θ' at the intersection point is given by

$$\theta'=\cos^{-1}\left(\frac{a}{c'}\left((a-c')\frac{1+\frac{c'}{a}}{a_0}-1\right)\right) \qquad (15.73).$$

346. The system of claim 345, wherein the angle $\theta_{A\,AO}$ the radial vector of the A AO makes with the internuclear axis is

$$\theta_{A\,AO} = 180° - \theta' \qquad (15.74).$$

347. The system of claim 345, wherein the distance from the point of intersection of the orbitals to the internuclear axis is the same for both component orbitals such that the angle $\omega t = \theta_{H_2MO}$ between the internuclear axis and the point of intersection of each H_2-type ellipsoidal MO with the A radial vector obeys the following relationship:

$$r_A \sin\theta_{A\,AO} = b \sin\theta_{H_2MO} \qquad (15.75)$$

such that

$$\theta_{H_2MO} = \sin^{-1}\frac{r_a \sin\theta_{A\,AO}}{b} \qquad (15.76).$$

348. The system of claim 347, wherein the distance d_{H_2MO} along the internuclear axis from the origin of H_2-type ellipsoidal MO to the point of intersection of the orbitals is given by

$$d_{H_2MO} = a\cos\theta_{H_2MO} \qquad (15.77).$$

349. The system of claim 347, wherein the distance $d_{A\,AO}$ along the internuclear axis from the origin of the A atom to the point of intersection of the orbitals is given by

$$d_{A\,AO} = c' - d_{H_2MO} \qquad (15.78).$$

350. The system of claim 1, wherein in ACB MO comprising a linear combination of $C-A$-bond and $C-B$-bond MOs where C is the general central atom and a bond is possible between the A and B atoms of the $C-A$ and $C-B$ bonds, the $\angle ACB$ bond angle is determined by the condition that the total energy of the H_2-type ellipsoidal MO between the terminal A and B atoms is zero.

351. The system of claim 350, wherein the force constant k' of a H_2-type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\varepsilon_o} \qquad (15.79)$$

where C_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the specie which is 0.75 (Eq. (13.59)) for a terminal $A-H$ (A is H or other atom) and 1

otherwise and C_2 is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the chemical bond and is equal to the corresponding factor of Eqs. (15.42) and (15.52).

352. The system of claim 351, wherein the distance from the origin of the MO to each focus c' of the $A-B$ ellipsoidal MO is given by:

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2C_1C_2 a}} = \sqrt{\frac{aa_0}{2C_1C_2}} \qquad (15.80).$$

353. The system of claim 351, wherein the internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2C_1C_2}} \qquad (15.81).$$

354. The system of claim 351, wherein the length of the semiminor axis of the prolate spheroidal $A-B$ MO $b=c$ is given by Eq. (15.4).

355. The system of claim 351, wherein the component energies and the total energy, $E_T(H_2MO)$, of the $A-B$ bond are given by the energy equations (Eqs. (11.207-11.212), (11.213-11.217), and (11.239)) of H_2 except that the terms based on charge are multiplied by c_{BO}, the bond-order factor which is 1 for a single bond and when the MO comprises n_1 equivalent single bonds as in the case of functional groups. c_{BO} is 4 for an independent double bond as in the case of the CO_2 and NO_2 molecules.

356. The system of claim 355, wherein the kinetic energy term is multiplied by c'_{BO} which is 1 for a single bond, 2 for a double bond, and 9/2 for a triple bond, the electron energy terms are multiplied by c_1, the fraction of the H_2-type ellipsoidal MO basis function of a terminal chemical bond which is 0.75 (Eq. (13.233)) for a terminal $A-H$ (A is H or other atom) and 1 otherwise.

357. The system of claim 355, wherein the electron energy terms are further multiplied by c_2', the hybridization or energy-matching factor that results in an equipotential energy match of the participating at least two atomic orbitals of each terminal bond.

358. The system of claim 350, wherein when $A-B$ comprises atoms other than H, $E_T\left(atom-atom, msp^3.AO\right)$, the energy component due to the AO or HO's charge donation to the terminal MO, is added to the other energy terms to give $E_T(H_2MO)$:

$$E_T(H_2MO)=\frac{-e^2}{8\pi\varepsilon_0 c'}\left[c_1c_2'\left(2c_{BO}-c'_{BO}\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]+E_T\left(atom-atom, msp^3.AO\right) \quad (15.82).$$

359. The system of claim 350, the radiation reaction force in the case of the vibration of $A-B$ in the transition state corresponds to the Doppler energy, E_D, given by Eq. (11.181) that is dependent on the motion of the electrons and the nuclei.

360. The system of claim 359, wherein the total energy that includes the radiation reaction of the $A-B$ MO is given by the sum of $E_T(H_2MO)$ (Eq. (15.82)) and $\overline{E}_{osc}$ given Eqs. (11.213-11.220), (11.231-11.236), and (11.239-11.240).

361. The system of claim 360, wherein the total energy $E_T\left(A-B\right)$ of the $A-B$ MO including the Doppler term is

$$E_T\left(A-B\right)=\left[\left(\frac{-e^2}{8\pi\varepsilon_0 c'}\left[c_1c_2'\left(2c_{BO}-c'_{BO}\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right]+E_T\left(atom-atom, msp^3.AO\right)\right)\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{c_{BO}\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o a^3}}{m_e}}}{m_ec^2}}\right]+\frac{1}{2}\hbar\sqrt{\frac{c_{BO}\frac{c_1c_2'e^2}{8\pi\varepsilon_o a^3}-\frac{c_{BO}e^2}{8\pi\varepsilon_o\left(a+c'\right)^3}}{\mu}}\right] \quad (15.83)$$

where C_{1o} is the fraction of the H_2-type ellipsoidal MO basis function of the oscillatory transition state of the $A-B$ bond which is 0.75 (Eq. (13.233)) in the case of H bonding to a central atom and 1 otherwise, C_{2o} is the factor that results in an equipotential energy match of

the participating at least two atomic orbitals of the transition state of the chemical bond, and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass of the nuclei given by Eq. (11.154).

362. The system of claim 361, wherein to match the boundary condition that the total energy of the $A-B$ ellipsoidal MO is zero, $E_T(A-B)$ given by Eq. (15.83) is set equal to zero and substitution of Eq. (15.81) into Eq. (15.83) gives

$$0 = \left[\left(\frac{-e^2}{8\pi\varepsilon_0 \sqrt{\frac{aa_0}{2C_1C_2}}} \left[c_1 c_2' \left(2c_{BO} - c'_{BO} \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1C_2}}}{a - \sqrt{\frac{aa_0}{2C_1C_2}}} - 1 \right] + E_T\left(atom - atom, msp^3.AO\right) \right) \right.$$
$$\left. \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\varepsilon_o a^3}}{m_e}}}{m_e c^2}} \right] + \frac{1}{2}\hbar \sqrt{\frac{c_{BO} \frac{c_1 c_2' e^2}{8\pi\varepsilon_o a^3} - \frac{c_{BO} e^2}{8\pi\varepsilon_o \left(a + \sqrt{\frac{aa_0}{2C_1C_2}} \right)^3}}{\mu}} \right] \quad (15.84).$$

363. The system of claim 362, wherein the vibrational energy-term of Eq. (15.84) is determined by the forces between the central field and the electrons and those between the nuclei (Eqs. (11.141-11.145)).

364. The system of claim 362, wherein the electron-central-field force and its derivative are given by

$$f(a) = -c_{BO} \frac{c_1 c_2' e^2}{4\pi\varepsilon_0 a^3} \quad (15.85)$$

and

$$f'(a) = 2c_{BO} \frac{c_1 c_2' e^2}{4\pi\varepsilon_0 a^3} \quad (15.86).$$

365. The system of claim 364, wherein the nuclear repulsion force and its derivative are given by

$$f(a+c') = \frac{e^2}{8\pi\varepsilon_o (a+c')^2} \quad (15.87)$$

and

$$f'(a+c') = -\frac{e^2}{4\pi\varepsilon_o (a+c')^3} \quad (15.88)$$

such that the angular frequency of the oscillation is given by

$$\omega = \sqrt{\frac{\left[\frac{-3}{a} f(a) - f'(a)\right]}{\mu}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO}\frac{c_1 c_2' e^2}{4\pi\varepsilon_0 a^3} - \frac{e^2}{8\pi\varepsilon_0 (a+c')^2}}{\mu}} \quad (15.89).$$

366. The system of claim 365, wherein since both terms of $\overline{E}_{osc} = \overline{E}_D + \overline{E}_{Kvib}$ are small due to the large values of a and c', an approximation of Eq. (15.84) which is evaluated to determine the bond angles of functional groups is given by

$$0 = \left[\left(\frac{-e^2}{8\pi\varepsilon_0\sqrt{\frac{aa_0}{2C_1C_2}}}\left[c_1c_2'\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2C_1C_2}}}{a-\sqrt{\frac{aa_0}{2C_1C_2}}} - 1\right] + E_T\left(atom-atom, msp^3.AO\right)\right)\right.$$
$$\left.\left[1+\sqrt{\frac{2\hbar\sqrt{\frac{\frac{c_1e^2}{4\pi\varepsilon_o a^3}}{m_e}}}{m_e c^2}}\right] + \frac{1}{2}\hbar\sqrt{\frac{\frac{c_1e^2}{8\pi\varepsilon_o a^3} - \frac{e^2}{8\pi\varepsilon_o\left(a+\sqrt{\frac{aa_0}{2C_1C_2}}\right)^3}}{\mu}}\right] \quad (15.90).$$

367. The system of claim 366, wherein from the energy relationship given by Eq. (15.90) and the relationship between the axes given by Eqs. (15.2-15.5), the dimensions of the $A-B$ MO can be solved.

368. The system of claim 367, wherein Eq. (15.90) is solved by the reiterative technique using a computer.

369. The system of claim 366, wherein a factor c_2 of a given atom in the determination of c_2' for calculating the zero of the total $A-B$ bond energy is given by Eqs. (15.62-15.65).

370. The system of claim 369, wherein in the case of a $H-H$ terminal bond of an alkyl or alkenyl group, c_2' is the ratio of c_2 of Eq. (15.62) for the $H-H$ bond which is one and c_2 of the carbon of the corresponding $C-H$ bond:

$$c_2' = \frac{1}{c_2(C2sp^3)} = \frac{13.605804\ eV}{E_{Coulomb}\left(C-H\ C2sp^3\right)} \qquad (15.91)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

371. The system of claim 366, wherein in the case of the determination of the bond angle of the ACH MO comprising a linear combination of $C-A$ -bond and $C-H$ -bond MOs where A and C are general, C is the central atom, and c_2 for an atom is given by Eqs. (15.62-15.70), c_2' of the $A-H$ terminal bond is the ratio of c_2 of the A atom for the $A-H$ terminal bond and c_2 of the C atom of the corresponding $C-H$ bond:

$$c_2' = \frac{c_2(A(A-H)msp^3)}{c_2(C(C-H)(msp^3)} \qquad (15.92).$$

372. The system of claim 366, wherein in the case of the determination of the bond angle of the COH MO of an alcohol comprising a linear combination of $C-O$-bond and $O-H$ -bond MOs where C, O, and H are carbon, oxygen, and hydrogen, respectively, c_2' of the $C-H$ terminal bond is 0.91771 since the oxygen and hydrogen atoms are at the Coulomb potential of a proton and an electron (Eqs. (1.236) and (10.162), respectively) that is energy matched to the $C2sp^3$ HO, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

373. The system of claim 366, wherein in the determination of the hybridization factor c_2' of Eq. (15.90) from Eqs. (15.62-15.70), the Coulombic energy, $E_{Coulomb}\left(MO.atom, msp^3\right)$, or the energy, $E\left(MO.atom, msp^3\right)$, the radius $r_{A-B\ AorBsp^3}$ of the A or B AO or HO of the heteroatom of the $A-B$ terminal bond MO such as the $C2sp^3$ HO of a terminal $C-C$

bond is calculated using Eq. (15.32) by considering $\sum E_{T_{mol}}\left(MO, 2sp^3\right)$, the total energy donation to each bond with which it participates in bonding as it forms the terminal bond.

374. The system of claim 373, wherein the Coulombic energy $E_{Coulomb}\left(MO.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by Eq. (15.19).

375. The system of claim 374, wherein in the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ (Eq. (15.15)) at the initial radius r of the AO electron, and the energy $E\left(MO.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(MO.atom, msp^3\right)$ and $E(magnetic)$ (Eq. (15.20)).

376. The system of claim 365, wherein in the specific case of the terminal bonding of two carbon atoms, the c_2 factor of each carbon given by Eq. (15.62) is determined using the Coulombic energy $E_{Coulomb}\left(C-C\ C2sp^3\right)$ of the outer electron of the $C2sp^3$ shell given by Eq. (15.19) with the radius $r_{C-C\ C2sp^3}$ of each $C2sp^3$ HO of the terminal $C-C$ bond calculated using Eq. (15.32) by considering $\sum E_{T_{mol}}\left(MO, 2sp^3\right)$, the total energy donation to each bond with which it participates in bonding as it forms the terminal bond including the contribution of the methylene energy, 0.92918 eV (Eq. (14.513)), corresponding to the terminal $C-C$ bond. The corresponding $E_T\left(atom-atom, msp^3.AO\right)$ in Eq. (15.90) is $E_T\left(C-C\ C2sp^3\right)=-1.85836\ eV$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

377. The system of claim 366, wherein in the case that the terminal atoms are carbon or other heteroatoms, the terminal bond comprises a linear combination of the HOs or AOs; thus, c_2' is the average of the hybridization factors of the participating atoms corresponding to the normalized linear sum:

$$c_2' = \frac{1}{2}\left(c_2'\left(atom\ 1\right) + c_2'\left(atom\ 2\right)\right) \qquad (15.93)$$

In the exemplary cases of $C-C$, $O-O$, and $N-N$ where C is carbon:

$$c_2' = \frac{1}{2}\left(\frac{\frac{e^2}{8\pi\varepsilon_0 a_0}}{\frac{e^2}{8\pi\varepsilon_0 r_{A-A\ A_1AO/HO}}} + \frac{\frac{e^2}{8\pi\varepsilon_0 a_0}}{\frac{e^2}{8\pi\varepsilon_0 r_{A-A\ A_2AO/HO}}}\right) \qquad (15.94)$$

$$= \frac{1}{2}\left(\frac{13.605804\ eV}{E_{Coulomb}\left(A-A.A_1AO/HO\right)} + \frac{13.605804\ eV}{E_{Coulomb}\left(A-A.A_2AO/HO\right)}\right)$$

In the exemplary cases of $C-N$, $C-O$, and $C-S$,

$$c_2' = \frac{1}{2}\left(\frac{13.605804\ eV}{E_{Coulomb}\left(C-B\ C2sp^3\right)} + c_2\left(C\ to\ B\right)\right) \qquad (15.95)$$

where C is carbon and $c_2\left(C\ to\ B\right)$ is the hybridization factor of Eqs. (15.52) and (15.84) that matches the energy of the atom B to that of the atom C in the group.

378. The system of claim 363, wherein the corresponding $E_T\left(atom-atom, msp^3.AO\right)$ term in Eq. (15.90) depends on the hybridization and bond order of the terminal atoms in the molecule, but typical values matching those used in the determination of the bond energies (Eq. (15.56)) are

$E_T\left(C-O\ C2sp^3.O2p\right) = -1.44915\ eV$; $E_T\left(C-O\ C2sp^3.O2p\right) = -1.65376\ eV$;

$E_T\left(C-N\ C2sp^3.N2p\right) = -1.44915\ eV$; $E_T\left(C-S\ C2sp^3.S2p\right) = -0.72457\ eV$;

$E_T\left(O-O\ O2p.O2p\right) = -1.44915\ eV$; $E_T\left(O-O\ O2p.O2p\right) = -1.65376\ eV$;

$E_T\left(N-N\ N2p.N2p\right) = -1.44915\ eV$; $E_T\left(N-O\ N2p.O2p\right) = -1.44915\ eV$;

$E_T\left(F-F\ F2p.F2p\right) = -1.44915\ eV$; $E_T\left(Cl-Cl\ Cl3p.Cl3p\right) = -0.92918\ eV$;

$E_T\left(Br-Br\ Br4p.Br4p\right) = -0.92918\ eV$; $E_T\left(I-I\ I5p.I5p\right) = -0.36229\ eV$;

$E_T\left(C-F\ C2sp^3.F2p\right) = -1.85836\ eV$; $E_T\left(C-Cl\ C2sp^3.Cl3p\right) = -0.92918\ eV$;

$E_T\left(C-Br\ C2sp^3.Br4p\right) = -0.72457\ eV$; $E_T\left(C-I\ C2sp^3.I5p\right) = -0.36228\ eV$, and

$E_T\left(O-Cl\ O2p.Cl3p\right) = -0.92918\ eV$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to + 10%, if desired.

379. The system of claim 366, wherein in the case that the terminal bond is $X-X$ where X is a halogen atom, c_1 is one, and c_2' is the average (Eq. (15.93)) of the hybridization factors of the participating halogen atoms given by Eqs. (15.62-15.63) where $E_{Coulomb}\left(MO.atom, msp^3\right)$ is determined using Eq. (15.32) and $E_{Coulomb}\left(MO.atom, msp^3\right)=13.605804\ eV$ for $X=I$.

380. The system of claim 379, wherein the factor C_1 of Eq. (15.90) is one for all halogen atoms.

381. The system of claim 379, wherein the factor C_2 of fluorine is one since it is the only halogen wherein the ionization energy is greater than that $13.605804\ eV$, the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

382. The system of claim 379, wherein for each of the halogens, Cl, Br, and I, C_2 is the hybridization factor of Eq. (15.52) given by Eq. (15.70) with $c_2(1)$ being that of the halogen given by Eq. (15.68) that matches the valence energy of X ($E_1\left(valence\right)$) to that of the $C2sp^3$ HO ($E_2\left(valence\right)=-14.63489\ eV$, Eq. (15.25)) and to the hybridization of $C2sp^3$ HO ($c_2(2)=0.91771$, Eq. (13.430)), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

383. The system of claim 382, wherein $E_T\left(atom-atom, msp^3.AO\right)$ of Eq. (15.90) is the maximum for the participating atoms which is $-1.44915\ eV$, $-0.92918\ eV$, $-0.92918\ eV$, and $-0.33582\ eV$ for F, Cl, Br, and I, respectively, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

384. The system of claim 366, wherein in the case that the terminal bond is $C-X$ where C is a carbon atom and X is a halogen atom, the factors c_1 and C_1 of Eq. (15.90) are one for all halogen atoms.

385. The system of claim 384, wherein for $X=F$, c_2' is the average (Eq. (15.95)) of the hybridization factors of the participating carbon and F atoms where c_2 for carbon is given by Eq. (15.62) and c_2 for fluorine matched to carbon is given by Eq. (15.70) with $c_2(1)$ for the fluorine atom given by Eq. (15.68) that matches the valence energy of F ($E_1(valence)=-17.42282\ eV$) to that of the $C2sp^3$ HO ($E_2(valence)=-14.63489\ eV$, Eq. (15.25)) and to the hybridization of $C2sp^3$ HO ($c_2(2)=0.91771$, Eq. (13.430)), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

386. The system of claim 385, wherein the factor C_2 of fluorine is one since it is the only halogen wherein the ionization energy is greater than that $13.605804\ eV$, the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

387. The system of claim 385, wherein for each of the other halogens, Cl, Br, and I, c_2' is the hybridization factor of the participating carbon atom since the halogen atom is energy matched to the carbon atom.

388. The system of claim 387, wherein the C_2 of the terminal-atom bond matches that used to determine the energies of the corresponding $C-X$ -bond MO.

389. The system of claim 388, wherein C_2 is the hybridization factor of Eq. (15.52) given by Eq. (15.70) with $c_2(1)$ for the halogen atom given by Eq. (15.68) that matches the valence energy of X ($E_1(valence)$) to that of the $C2sp^3$ HO ($E_2(valence)=-14.63489\ eV$, Eq. (15.25)) and to the hybridization of $C2sp^3$ HO

($c_2(2) = 0.91771$, Eq. (13.430)), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

390. The system of claim 385, wherein $E_T\left(atom-atom, msp^3.AO\right)$ of Eq. (15.90) is the maximum for the participating atoms which is $-1.85836\ eV$, $-0.92918\ eV$, $-0.72457\ eV$, and $-0.33582\ eV$ for F, Cl, Br, and I, respectively, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

391. The system of claim 385, wherein in the case that the terminal bond is $H-X$ corresponding to the angle of the atoms HCX where C is a carbon atom and X is a halogen atom, the factors c_1 and C_1 of Eq. (15.90) are 0.75 for all halogen atoms.

392. The system of claim 385, wherein for $X = F$, c_2' is given by Eq. (15.69) with c_2 of the participating carbon and F atoms given by Eq. (15.62) and Eq. (15.65), respectively.

393. The system of claim 392, wherein the factor C_2 of fluorine is one since it is the only halogen wherein the ionization energy is greater than that $13.605804\ eV$, the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

394. The system of claim 393, wherein for each of the other halogens, Cl, Br, and I, c_2' is also given by Eq. (15.69) with c_2 of the participating carbon given by Eq. (15.62) and c_2 of the participating X atom given by $c_2 = 0.91771$ (Eq. (13.430)) since the X atom is energy matched to the $C2sp^3$ HO.

395. The system of claim 394, wherein C_2 is given by Eq. (15.65) for the corresponding atom X where C_2 matches the energy of the atom X to that of H.

396. The system of claim 366, wherein the distance between the two atoms A and B of the general molecular group ACB when the total energy of the corresponding $A-B$ MO is zero, the corresponding bond angle can be determined from the law of cosines:

$$s_1^2 + s_2^2 - 2s_1 s_2 \text{cosine}\theta = s_3^2 \quad (15.96).$$

397. The system of claim 396, wherein with $s_1 = 2c'_{C-A}$, the internuclear distance of the $C-A$ bond, $s_2 = 2c'_{C-B}$, the internuclear distance of each $C-B$ bond, and $s_3 = 2c'_{A-B}$, the internuclear distance of the two terminal atoms, the bond angle $\theta_{\angle ACB}$ between the $C-A$ and $C-B$ bonds is given by

$$(2c'_{C-A})^2 + (2c'_{C-B})^2 - 2(2c'_{C-A})(2c'_{C-B})\text{cosine}\theta = (2c'_{A-B})^2 \quad (15.97)$$

$$\theta_{\angle ACB} = \cos^{-1}\left(\frac{(2c'_{C-A})^2 + (2c'_{C-B})^2 - (2c'_{A-B})^2}{2(2c'_{C-A})(2c'_{C-B})}\right) \quad (15.98).$$

398. The system of claim 397, wherein the structure $C_b C_a(O_a)O_b$ wherein C_a is bound to C_b, O_a, and O_b, the three bonds are coplanar and two of the angles are known, say θ_1 and θ_2, then the third θ_3 can be determined geometrically:

$$\theta_3 = 360 - \theta_1 - \theta_2 \quad (15.99)$$

399. The system of claim 397, wherein in the general case that two of the three coplanar bonds are equivalent and one of the angles is known, say θ_1, then the second and third can be determined geometrically:

$$\theta_2 = \theta_3 = \frac{(360 - \theta_1)}{2} \quad (15.100).$$

400. The system of claim 1, wherein in the general case where the group comprises three $A-B$ bonds having B as the central atom at the apex of a pyramidal structure formed by the three bonds with the A atoms at the base in the xy-plane.

401. The system of claim 400, wherein the C_{3v} axis centered on B is defined as the vertical or z-axis, and any two $A-B$ bonds form an isosceles triangle, and the angle of

the bonds and the distances from and along the z-axis are determined from the geometrical relationships given by Eqs. (13.412-13.416):

the distance $d_{origin-B}$ from the origin to the nucleus of a terminal B atom is given by

$$d_{origin-B} = \frac{2c'_{B-B}}{2\sin 60°} \quad (15.101)$$

the height along the z-axis from the origin to the A nucleus d_{height} is given by

$$d_{height} = \sqrt{\left(2c'_{A-B}\right)^2 - \left(d_{origin-B}\right)^2}, \text{ and } (15.102)$$

the angle θ_v of each $A-B$ bond from the z-axis is given by

$$\theta_v = \tan^{-1}\left(\frac{d_{origin-B}}{d_{height}}\right) \quad (15.103).$$

402. The system of claim 401, wherein in the case where the central atom B is further bound to a fourth atom C and the $B-C$ bond is along the z-axis. Then, the bond $\theta_{\angle ABC}$ given by Eq. (14.206) is

$$\theta_{\angle ABC} = 180 - \theta_v \quad (15.104).$$

403. The system of claim 400, wherein in the plane defined by a general ACA MO comprising a linear combination of two $C-A$-bond MOs where C is the central atom, the dihedral angle $\theta_{\angle BC/ACA}$ between the ACA-plane and a line defined by a third bond with C, specifically that corresponding to a $C-B$-bond MO, is calculated from the bond angle $\theta_{\angle ACA}$ and the distances between the A, B, and C atoms.

404. The system of claim 403, wherein the distance d_1 along the bisector of $\theta_{\angle ACA}$ from C to the internuclear-distance line between A and A, $2c'_{A-A}$, is given by

$$d_1 = 2c'_{C-A}\cos\frac{\theta_{\angle ACA}}{2} \quad (15.105)$$

where $2c'_{C-A}$ is the internuclear distance between A and C.

405. The system of claim 404, wherein the atoms A, A, and B define the base of a pyramid.

406. The system of claim 405, wherein the pyramidal angle $\theta_{\angle ABA}$ can be solved from the internuclear distances between A and A, $2c'_{A-A}$, and between A and B, $2c'_{A-B}$, using the law of cosines (Eq. (15.98)):

$$\theta_{\angle ABA} = \cos^{-1}\left(\frac{(2c'_{A-B})^2 + (2c'_{A-B})^2 - (2c'_{A-A})^2}{2(2c'_{A-B})(2c'_{A-B})}\right) \quad (15.106).$$

407. The system of claim 406, wherein the distance d_2 along the bisector of $\theta_{\angle ABA}$ from B to the internuclear-distance line $2c'_{A-A}$, is given by

$$d_2 = 2c'_{A-B}\cos\frac{\theta_{\angle ABA}}{2} \quad (15.107).$$

408. The system of claim 407, wherein the lengths d_1, d_2, and $2c'_{C-B}$ define a triangle wherein the angle between d_1 and the internuclear distance between B and C, $2c'_{C-B}$, is the dihedral angle $\theta_{\angle BC/ACA}$ that can be solved using the law of cosines (Eq. (15.98)):

$$\theta_{\angle BC/ACA} = \cos^{-1}\left(\frac{d_1^2 + (2c'_{C-B})^2 - d_2^2}{2d_1(2c'_{B-C})}\right) \quad (15.108).$$

409. The system of claim 1, wherein the specie are solved using the solutions of organic chemical functional groups as basis elements wherein the structures and energies where linearly added to achieve the molecular solutions, each functional group can be treated as a building block to form any desired molecular solution from the corresponding linear combination, each functional group element was solved using the atomic orbital and hybrid orbital spherical orbitsphere solutions bridged by molecular orbitals comprised of the H_2-type prolate spheroidal solution given in the Nature of the Chemical Bond of Hydrogen-Type Molecules section, the energy of each MO was matched at the HO or AO by matching the hybridization and total energy of the MO to the AOs and HOs, the energy E_{mag} (e.g. given by Eq. (15.58)) for a $C2sp^3$ HO and Eq.(15.59) for an $O2p$ AO) was subtracted for each set of unpaired electrons created by bond breakage.

410. They system of claim 409, wherein the bond energy is not equal to the component energy of each bond as it exists in the specie, although, they are close.

411. The system of claim 409, wherein the total energy of each group is its contribution to the total energy of the specie as a whole.

412. The system of claim 409, wherein the determination of the bond energies for the creation of the separate parts must take into account the energy of the formation of any radicals and any redistribution of charge density within the pieces and the corresponding energy change with bond cleavage.

413. The system of claim 409, wherein the vibrational energy in the transition state is dependent on the other groups that are bound to a given functional group, which will effect the functional-group energy, however because the variations in the energy based on the balance of the molecular composition are typically of the order of a few hundreds of electron volts at most, they are neglected.

414. The system of claim 409, wherein the energy of each functional-group MO bonding to a given carbon HO is independently matched to the HO by subtracting the contribution to the change in the energy of the HO from the total MO energy given by the sum of the MO contributions and $E\left(C,2sp^3\right)=-14.63489\ eV$ (Eq. (13.428)).

415. The system of claim 409, wherein the intercept angles are determined from Eqs. (15.71-15.78) using the final radius of the HO of each atom.

416. The system of claim 409, wherein a final carbon-atom radius is determined using Eqs. (15.32) wherein the sum of the energy contributions of each atom to all the MOs in which it participates in bonding is determined.

417. The system of claim 416, wherein the final radius is used in Eqs. (15.19) and (15.20) to calculate the final valence energy of the HO of each atom at the corresponding final radius.

418. The system of claim 417, wherein the radius of any bonding heteroatom that contributes to a MO is calculated in the same manner, and the energy of its outermost shell is matched to that of the MO by the hybridization factor between the carbon-HO energy and the energy of the heteroatomic shell.

419. The system of claim 416, wherein the donation of electron density to the AOs and HOs reduces the energy.

420. The system of claim 419, wherein the donation of the electron density to the MO's at each AO or HO is that which causes the resulting energy to be divided equally between the participating AOs or HOs to achieve energy matching.

421. The system of claim 1, wherein the molecular solutions are used to design synthetic pathways and predict product yields based on equilibrium constants calculated from the heats of formation.

422. The system of claim 1, wherein the new stable compositions of matter are predicted as well as the structures of combinatorial chemistry reactions.

423. The system of claim 1, wherein pharmaceutical applications include the ability to graphically or computationally render the structures of drugs that permit the identification of the biologically active parts of the specie to be identified from the common spatial charge-density functions of a series of active species.

424. The system of claim 1, wherein novel drugs are designed according to geometrical parameters and bonding interactions with the data of the structure of the active site of the drug.

425. The system of claim 1, wherein to calculate conformations, folding, and physical properties, the exact solutions of the charge distributions in any given specie are used to calculate the fields, and from the fields, the interactions between groups of the same specie or between groups on different species are calculated wherein the interactions are distance and relative orientation dependent.

426. The system of claim 425, the fields and interactions can be determined using a finite-element-analysis approach of Maxwell's equations.

427. The system of claim 1, wherein in the case where three sets of $C=C$-bond MOs form bonds between the two carbon atoms of each molecule to form a six-member ring such that the six resulting bonds comprise eighteen paired electrons, and each bond comprises a linear combination of two MOs wherein each comprises two $C2sp^3$ HOs and 75% of a H_2-type ellipsoidal MO divided between the $C2sp^3$ HOs:

$$\begin{pmatrix} 3\left(2\ C2sp^3 + 0.75\ H_2\ MO\right) \rightarrow 3\left(\overset{4e}{C=C}\right) - ethylene - type - bond\ MO \\ \rightarrow 6\left(\overset{3e}{C=C}\right) - bond\ MO\ of\ benzene \end{pmatrix} \quad (15.142).$$

428. The system of claim 427, wherein the linear combination of each H_2-type ellipsoidal MO with each $C2sp^3$ HO further comprises an excess 25% charge-density contribution per bond from each $C2sp^3$ HO to the $C=C$-bond MO to achieve an energy minimum.

429. The system of claim 427, wherein the dimensional parameters of each bond $C=C$-bond are determined using Eqs. (15.42) and (15.1-15.5) in a form that are the same equations as those used to determine the same parameters of the $C=C$-bond MO of ethylene (Eqs. (14.242-14.268)) while matching the boundary conditions of the structure of benzene.

430. The system of claim 427, wherein hybridization with 25% electron donation to each $C=C$-bond gives rise to the $C_{benzene}2sp^3$ HO-shell Coulombic energy $E_{Coulomb}\left(C_{benzene}, 2sp^3\right)$ given by Eq. (14.245).

431. The system of claim 427, wherein to meet the equipotential condition of the union of the six $C2sp^3$ HOs, c_2 and C_2 of Eq. (15.42) for the aromatic $\overset{3e}{C=C}$-bond MO is given by Eq. (15.62) as the ratio of 15.95955 eV, the magnitude of $E_{Coulomb}\left(C_{benzene}, 2sp^3\right)$ (Eq.

(14.245)), and 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of H (Eq. (1.243)):

$$C_2\left(benzeneC2sp^3HO\right)=c_2\left(benzeneC2sp^3HO\right)=\frac{13.605804\ eV}{15.95955\ eV}=0.85252 \quad (15.143)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

432. The system of claim 427, wherein the energies of each $C\overset{3e}{=}C$ bond of benzene are determined using the same equations as those of ethylene (Eqs. (14.251-14.253) and (14.319-14.333) with the parameters of benzene.

433. The system of claim 427, wherein ethylene serves as a basis element for the $C\overset{3e}{=}C$ bonding of benzene wherein each of the six $C\overset{3e}{=}C$ bonds of benzene comprises $(0.75)(4)=3$ electrons according to Eq. (15.142).

434. The system of claim 427, wherein the total energy of the bonds of the eighteen electrons of the $C\overset{3e}{=}C$ bonds of benzene, $E_T\left(C_6H_6,C\overset{3e}{=}C\right)$, is given by $(6)(0.75)$ times $E_{T+osc}(C=C)$ (Eq. (14.492)), the total energy of the $C\overset{3e}{=}C$-bond MO of benzene including the Doppler term, minus eighteen times $E\left(C,2sp^3\right)$ (Eq. (14.146)), the initial energy of each $C2sp^3$ HO of each C that forms the $C\overset{3e}{=}C$ bonds of bond order two.

435. The system of claim 427, wherein the total energy of the six $C\overset{3e}{=}C$ bonds of benzene with three electron per aromatic bond given by Eq. (14.493) is

$$\begin{aligned}E_T\left(C_6H_6,C\overset{3e}{=}C\right)&=(6)(0.75)E_{T+osc}(C=C)-(6)(3)E\left(C,2sp^3\right)\\&=(6)(0.75)(-66.05796\ eV)-18(-14.63489\ eV)\\&=-297.26081\ eV-(-263.42798\ eV)\\&=-33.83284\ eV\end{aligned} \quad (15.144)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

436. The system of claim 427, wherein the results of benzene can be generalized to the class of aromatic and heterocyclic compounds. $E_{h\nu}$ of an aromatic bond is given by $E_T\left(H_2\right)$ (Eqs. (11.212) and (14.486)), the maximum total energy of each H_2-type MO such that

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(-31.63536831\ eV\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right) \qquad (15.145),$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

437. The system of claim 435, wherein the factor of 0.75 corresponding to the three electrons per aromatic bond of bond order two given in the Benzene Molecule (C_6H_6) section modifies Eqs. (15.52-15.56).

438. The system of claim 437, wherein the multiplication of the total energy given by Eq. (15.55) by $f_1 = 0.75$ with the substitution of Eq. (15.145) gives the total energy of the aromatic bond:

$$E_T\left(Group\right) = f_1\left(\begin{array}{l} E(basis\ energies) + E_T\left(atom - atom, msp^3.AO\right) \\ -31.63536831\ eV\sqrt{\dfrac{2\hbar\sqrt{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}{m_e}}{m_e c^2}} + n_1\overline{E}_{Kvib} + c_3\dfrac{8\pi\mu_o\mu_B^2}{r^3} \end{array}\right) \qquad (15.146)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

439. The system of claim 427, wherein the total bond energy of the aromatic group $E_D\left(Group\right)$ is the negative difference of the total energy of the group (Eq. (15.146)) and the

total energy of the starting species given by the sum of $c_4 E_{initial}\left(c_4\ AO/HO\right)$ and $c_5 E_{initial}\left(c_5\ AO/HO\right)$:

$$E_D(Group) = -\left(f_1\left(\begin{array}{l} E(basis\ energies) + E_T\left(atom-atom, msp^3.AO\right) \\ -31.63536831\ eV\sqrt{\dfrac{2\hbar\sqrt{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}{m_e}}{m_e c^2}} + n_1\bar{E}_{Kvib} + c_3\dfrac{8\pi\mu_o\mu_B^2}{r^3} \\ -\left(c_4 E_{initial}\left(AO/HO\right) + c_5 E_{initial}\left(c_5\ AO/HO\right)\right) \end{array} \right) \right)$$

(15.147), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

440. The system of claim 427, wherein benzene is considered as comprising chemical bonds between six CH radicals wherein each radical comprises a chemical bond between carbon and hydrogen atoms, energy components of V_e, V_p, T, V_m, and E_T are the same as those of the hydrogen carbide radical, except that $E_T\left(C=C, 2sp^3\right) = -1.13379\ eV$ (Eq. (14.247)) is subtracted from $E_T(CH)$ of Eq. (13.495) to match the energy of each $C-H$-bond MO to the decrease in the energy of the corresponding $C2sp^3$ HO, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

441. The system of claim 440, wherein in the corresponding generalization of the aromatic CH group, the geometrical parameters are determined using Eq. (15.42) and Eqs. (15.1-15.5) with $E_T\left(atom-atom, msp^3.AO\right) = -1.13379\ eV$ wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to ± 10%, if desired.

442. The system of claim 440, wherein the total energy of the benzene $C-H$-bond MO, $E_{T_{benzene}}\left(C-H\right)$, given by Eq. (14.467) is the sum of $0.5E_T\left(C=C, 2sp^3\right)$, the energy change of each $C2sp^3$ shell per single bond due to the decrease in radius with the

formation of the corresponding $C\overset{3e}{=}C$-bond MO (Eq. (14.247)), and $E_{T_{benzene}}(CH)$, the σ MO contribution given by Eq. (14.441). In the corresponding generalization of the aromatic CH group, the energy parameters are determined using Eqs. (15.146-15.147) with $f_1 = 1$ and $E_T(atom - atom, msp^3.AO) = \frac{-1.13379\ eV}{2}$, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

443. The system of claim 442, wherein the energy contribution to the single aromatic CH bond is one half that of the $C\overset{3e}{=}C$ double bond contribution, which matches the energies of the CH and $C\overset{3e}{=}C$ aromatic groups, conserves the electron number with the equivalent charge density as that of $s = 1$ in Eqs. (15.18-15.21), and further gives a minimum energy for the molecule.

444. The system of claim 443, wherein the breakage of the aromatic $C\overset{3e}{=}C$ bonds to give CH groups creates unpaired electrons in these fragments that corresponds to $c_3 = 1$ in Eq. (15.56) with E_{mag} given by Eq. (15.58).

445. The system of claim 444, wherein each of the $C - H$ bonds of benzene comprises two electrons according to Eq. (14.439).

446. The system of claim 445, wherein from the energy of each $C - H$ bond, $-E_{D_{benzene}}(^{12}CH)$ (Eq. (14.477)), the total energy of the twelve electrons of the six $C - H$ bonds of benzene, $E_T(C_6H_6, C - H)$, given by Eq. (14.494) is

$$E_T(C_6H_6, C - H) = (6)(-E_{D_{benzene}}(^{12}CH)) = 6(-3.90454\ eV) = -23.42724\ eV$$

(15.148), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

447. The system of claim 440, wherein the total bond dissociation energy of benzene, $E_D\left(C_6H_6\right)$, given by Eq. (14.495) is the negative sum of $E_T\left(C_6H_6,C\overset{3e}{=}C\right)$ (Eq. (14.493)) and $E_T\left(C_6H_6,C-H\right)$ (Eq. (14.494)):

$$\begin{aligned} E_D\left(C_6H_6\right) &= -\left(E_T\left(C_6H_6,C\overset{3e}{=}C\right)+E_T\left(C_6H_6,C-H\right)\right) \\ &= -\left(\left(-33.83284\ eV\right)+\left(-23.42724\ eV\right)\right) \\ &= 57.2601\ eV \end{aligned} \qquad (15.149)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to $\pm$ 10%, if desired.

448. The system of claim 447, wherein using the parameters given in Tables 15.214 and 15.216 in the general equations (Eqs. (15.42), (15.1-15.5), and (15.146-15.147)) reproduces the results for benzene given in the Benzene Molecule (C_6H_6) section as shown in Tables 15.214 and 15.216.

449. A system of computing and rendering the nature of at least one specie selected from a group of diatomic molecules having at least one atom that is other than hydrogen, polyatomic molecules, molecular ions, polyatomic molecular ions, or molecular radicals, or any functional group therein, comprising physical, Maxwellian solutions of charge, mass, and current density functions of said specie, said system comprising:

processing means for processing physical, Maxwellian equations representing charge, mass, and current density functions of said specie to produce at least one Maxwellian solution; and

an output means for outputting the Maxwellian solution.

450. The system of claim 449, further comprising a data transfer system for inputting numerical data into or out of a computational components and storage components of the main system.

451. The system of claim 449, further comprising a spreadsheet containing solutions of the bond parameters with output in a standard spreadsheet format.

452. The system of claim 451, further comprising a data-handling program to transfer data from the spreadsheets into the main program.

453. The system of claim 449, wherein output may be at least one of graphical, simulation, text, and numerical data.

454. The system of claim 453, wherein the output may be the calculation of at least one of: (1) a bond distance between two of the atoms; (2) a bond angle between three of the atoms; (3) a bond energy between two of the atoms; (4) orbital intercept distances and angles; and (5) charge-density functions of atomic, hybridized, and molecular orbitals, wherein the bond distance, bond angle, and bond energy are calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration

455. The system of claim 449, wherein the charge, current, energy, and geometrical parameters are output to be inputs to other programs that can be used in further applications.

456. The system of claim 455, wherein the data of heats of formation can be input to another program to be used to predict stability (existence of compounds) equilibrium constants and to predict synthetic pathways.

457. The system of claim 456, wherein novel composition of matters can be discovered by calculating at least one of a bond distance between two of the atoms, a bond angle between three of the atoms, and a bond energy between two of the atoms, orbital intercept distances and angles, charge-density functions of atomic, hybridized, and molecular orbitals, the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.

458. The system of claim 456, wherein the charge and current density functions can be used to predict the electric and magnetic fields of the species to determine other properties due to the interaction of the fields between species.

459. The system of claim 458, wherein finite-element analysis is used to predict or calculate the interaction and resulting properties, such as the freezing point, boiling point, density, viscosity, and refractive index.

460. The system of claim 449, wherein the output data can be used to give thermodynamic, spectroscopic, and other properties, aid in drug design and other applications with or without direct visualization.

461. The system of claim 449, wherein the data can be input into other programs of the system, which calculate thermodynamic and other properties, or performs a simulation, such as a chemical reaction or molecular dynamics.

462. A method of using any of the systems or compositions of matter of claims 1-461.

463. A use of any system or composition of matter of claims 1-461.

Fig.1

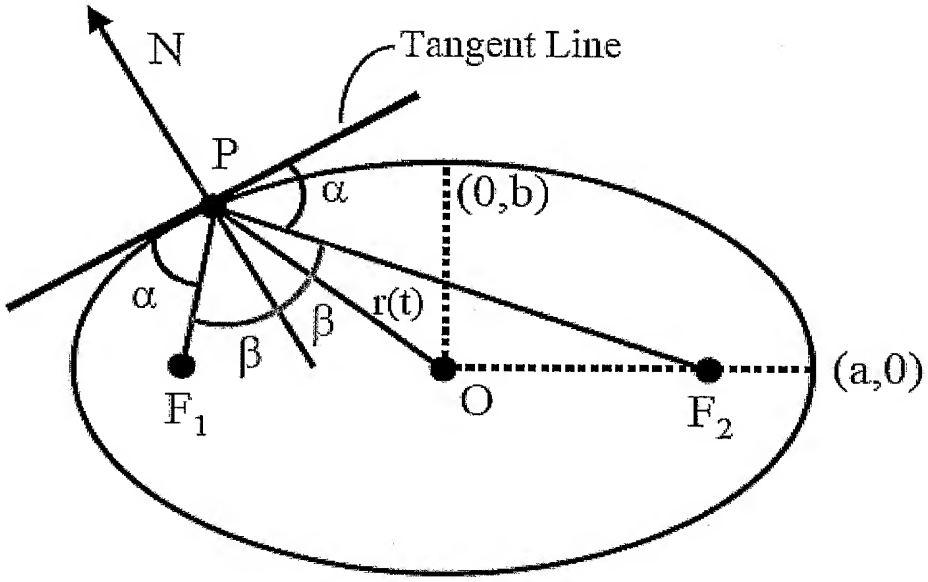


Fig.2

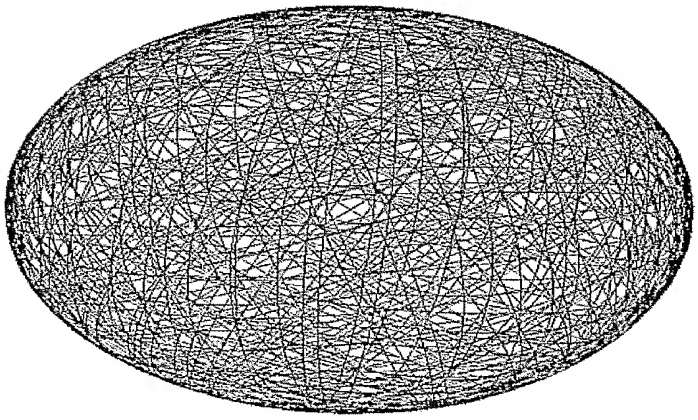


Fig.3

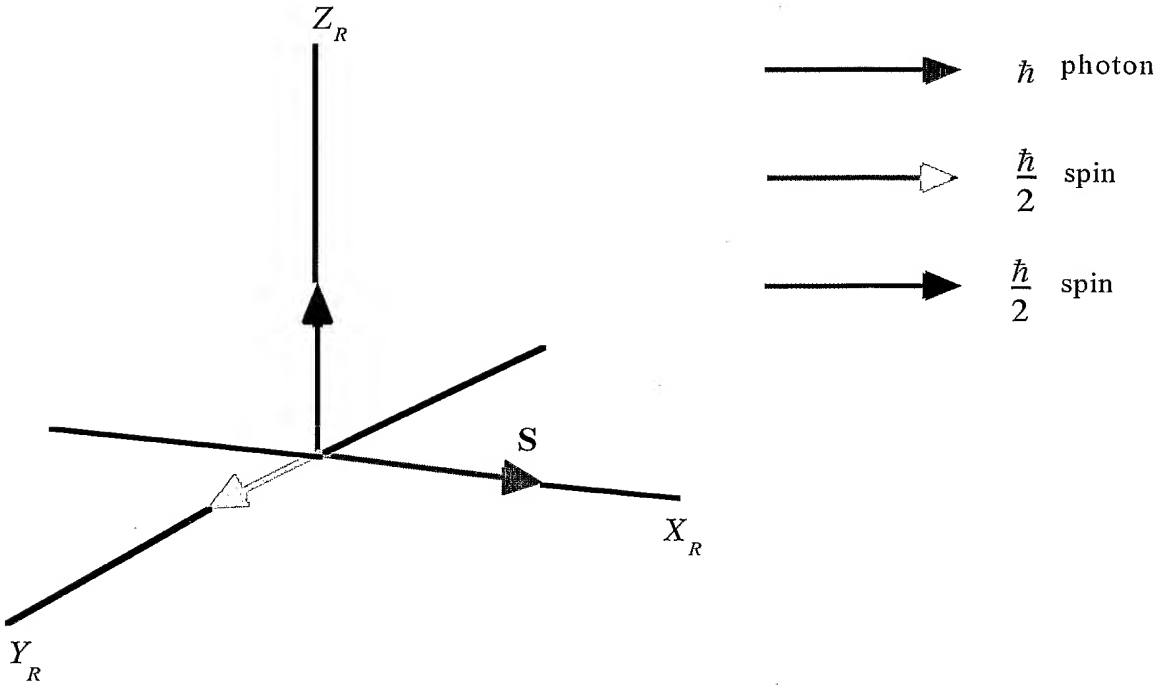


Fig.4

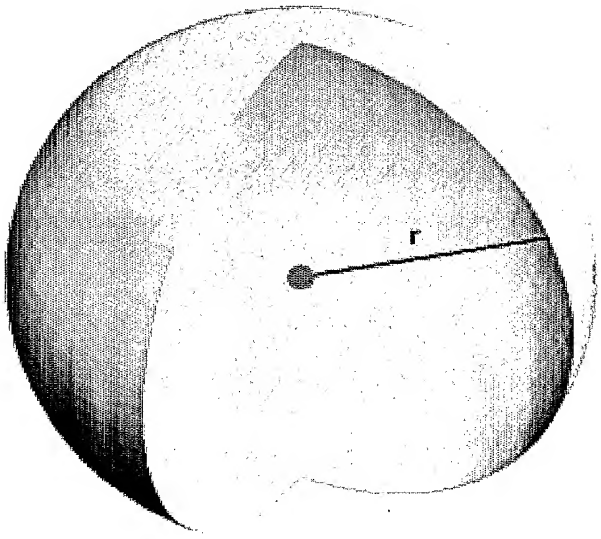
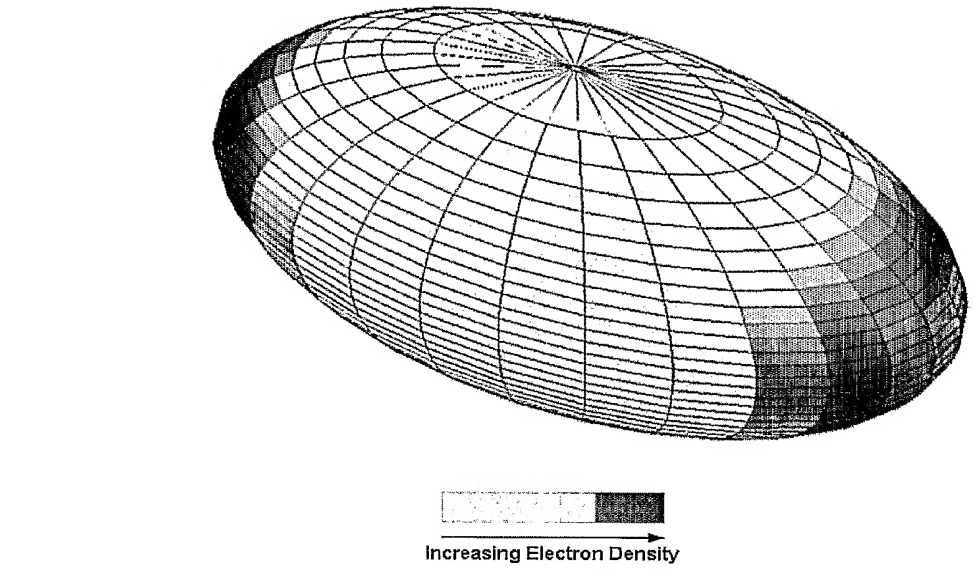
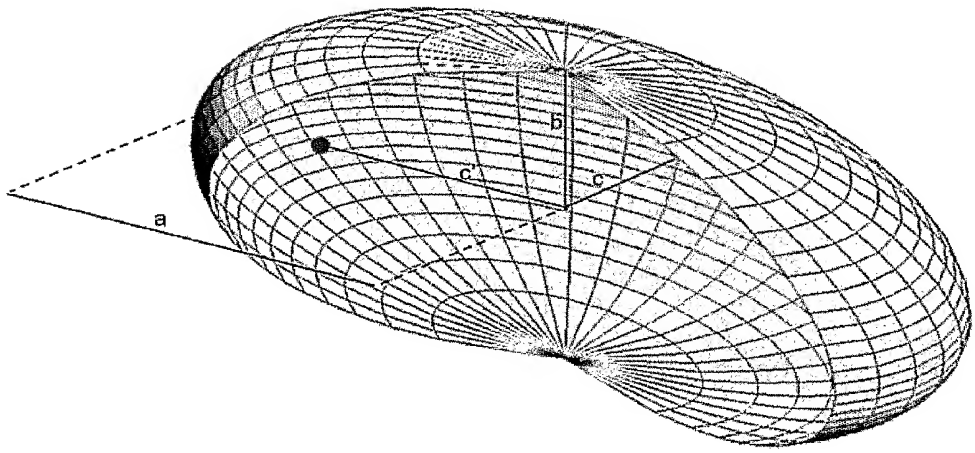


Fig.5



A



B

Fig. 6

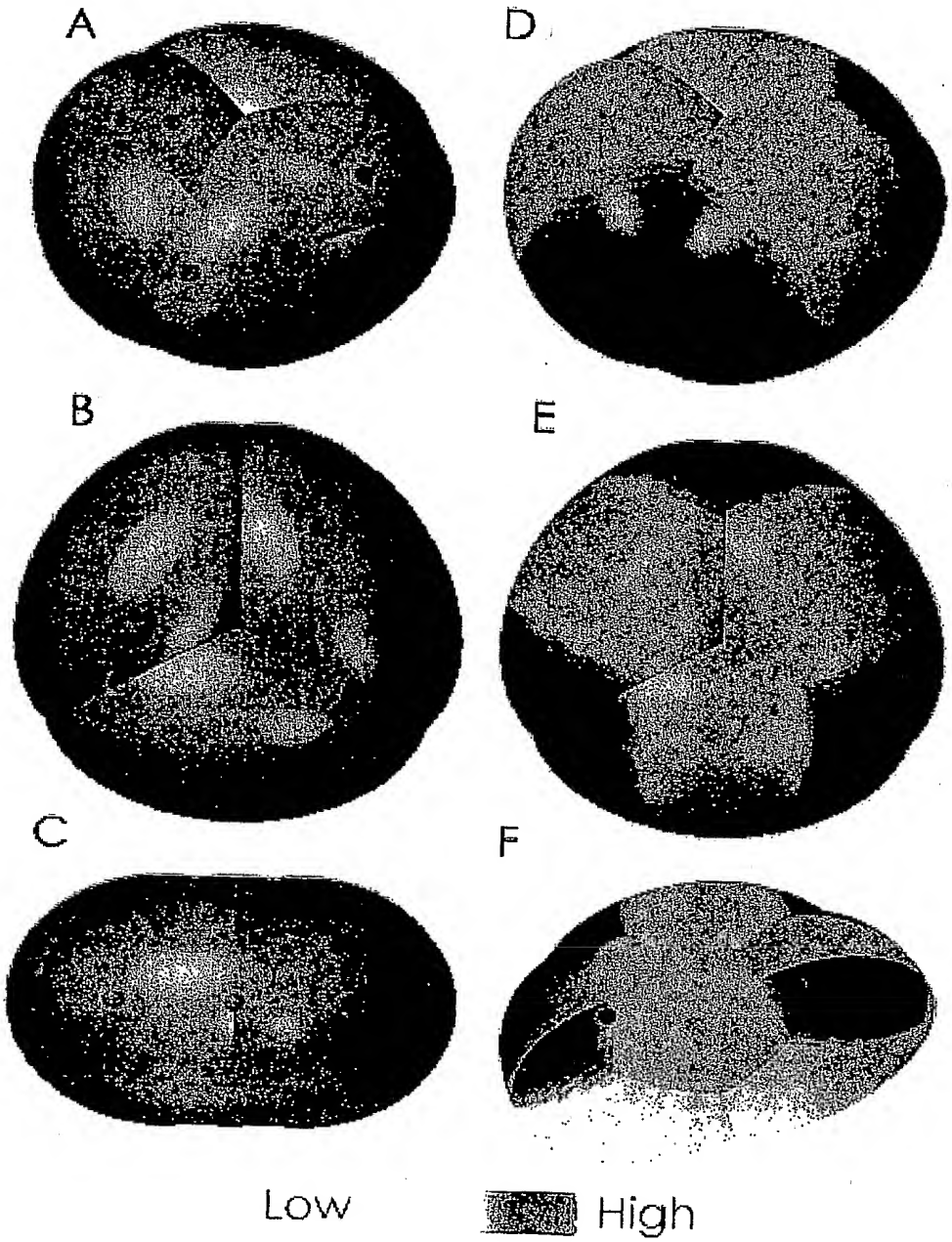


Fig.7

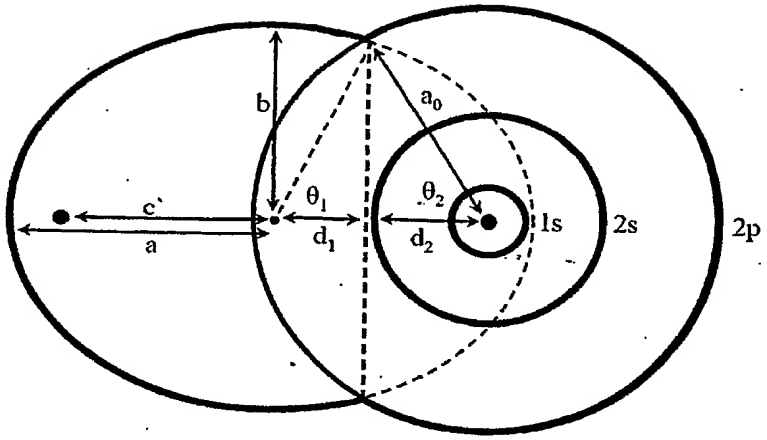


Fig.8

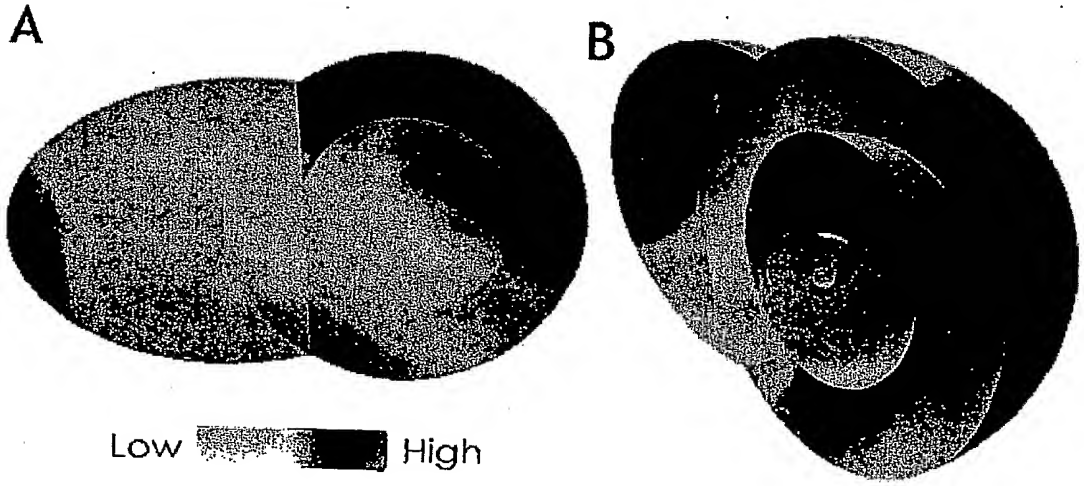


Fig.9

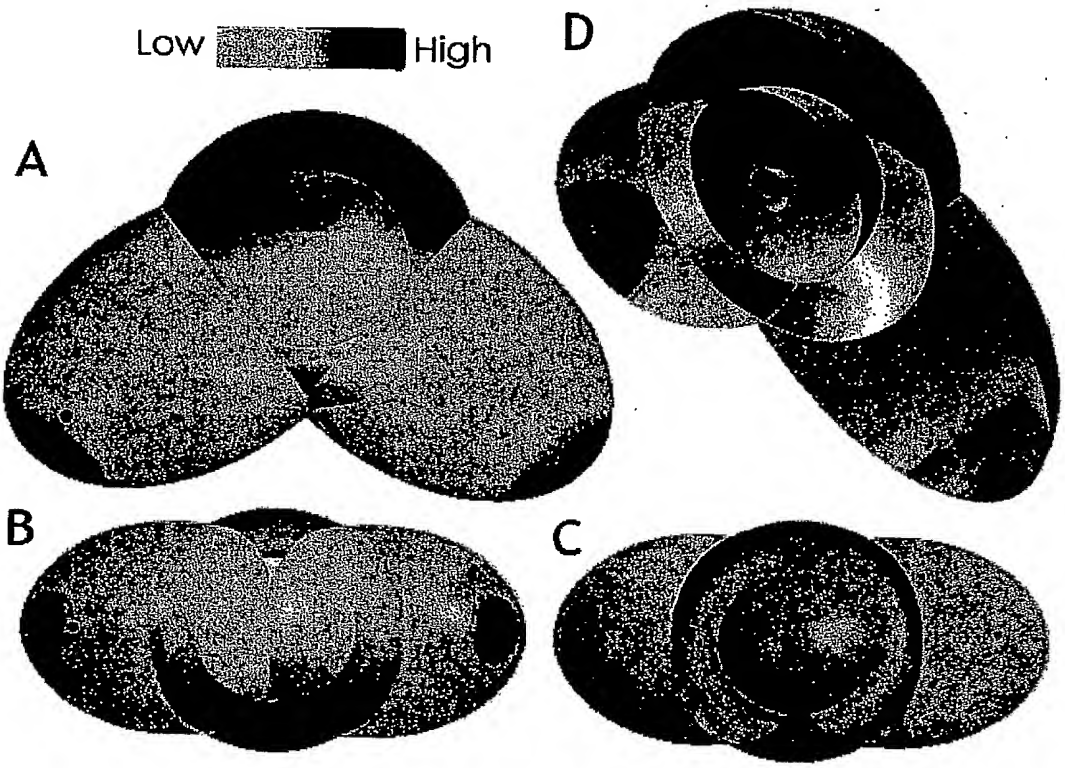


Fig.10

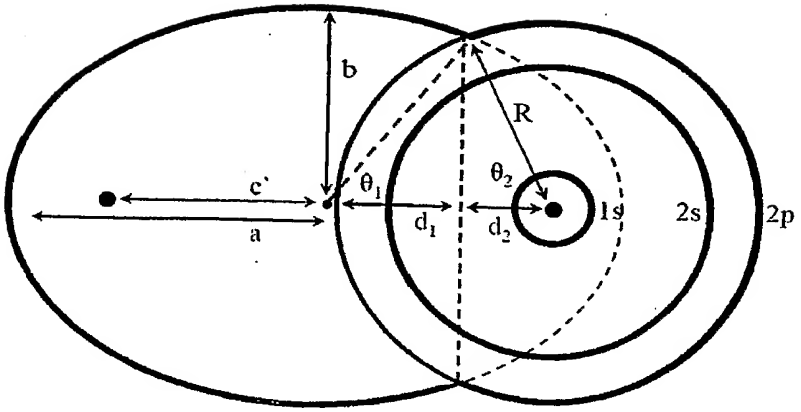


Fig.11

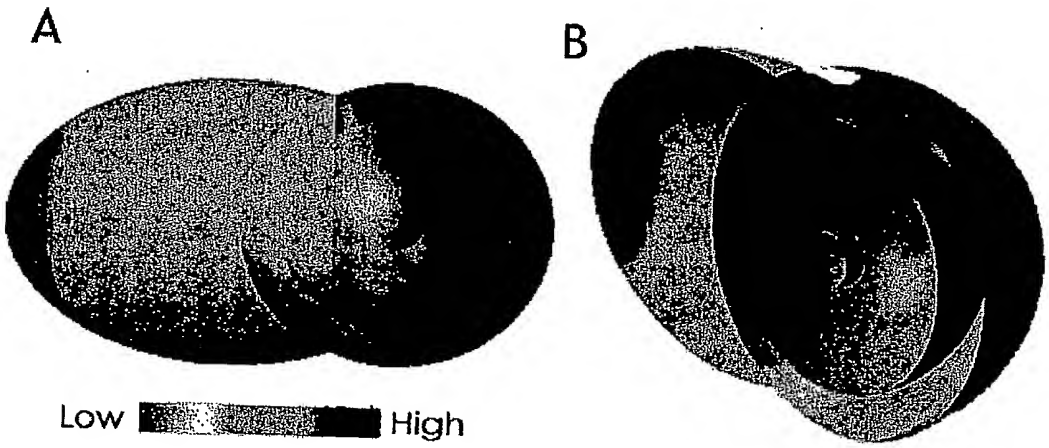


Fig.12

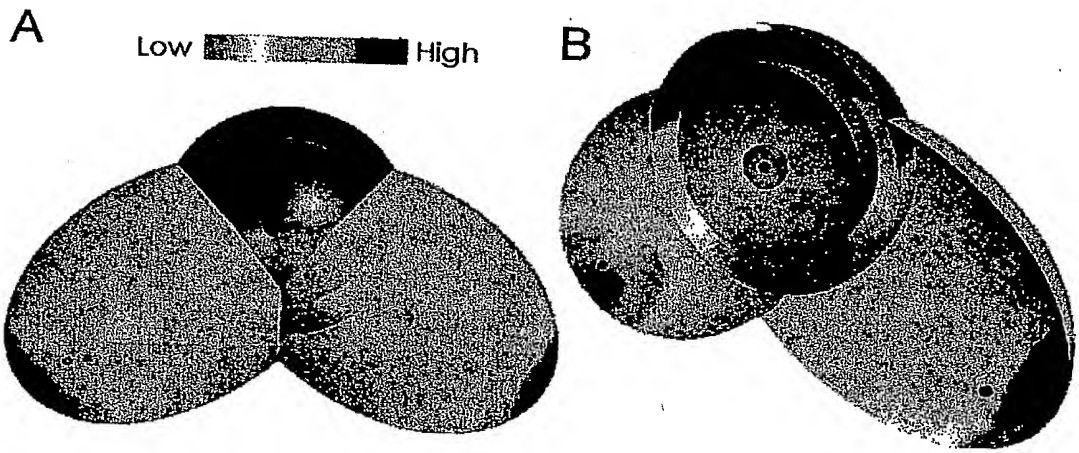


Fig. 13

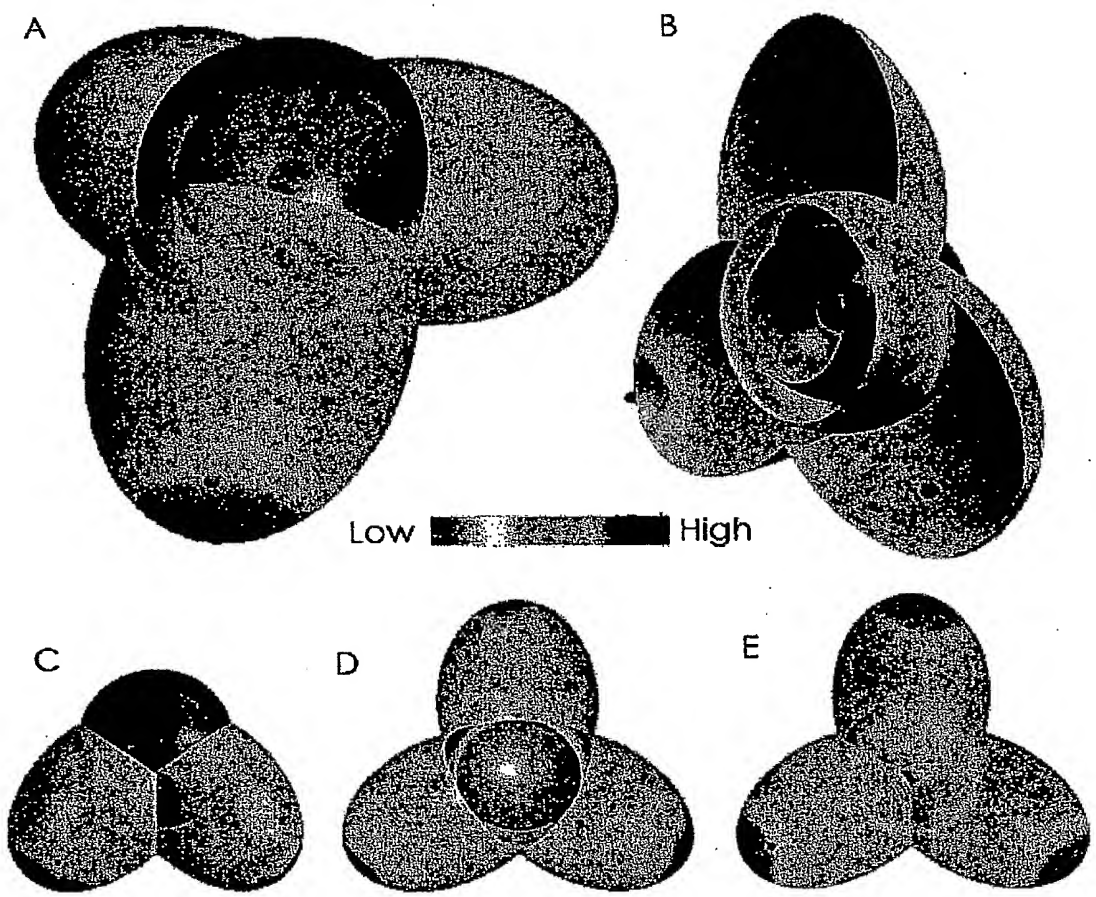


Fig.14

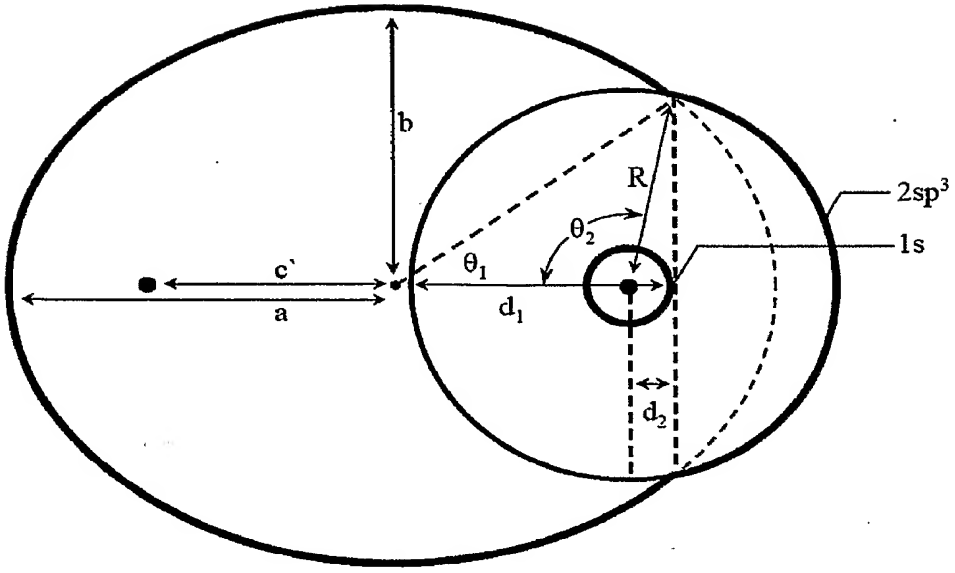


Fig.15

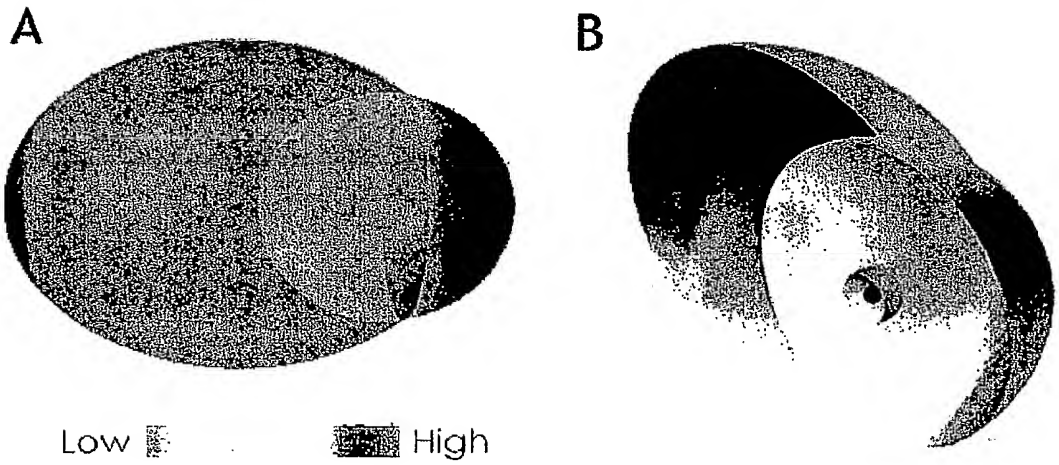


Fig.16

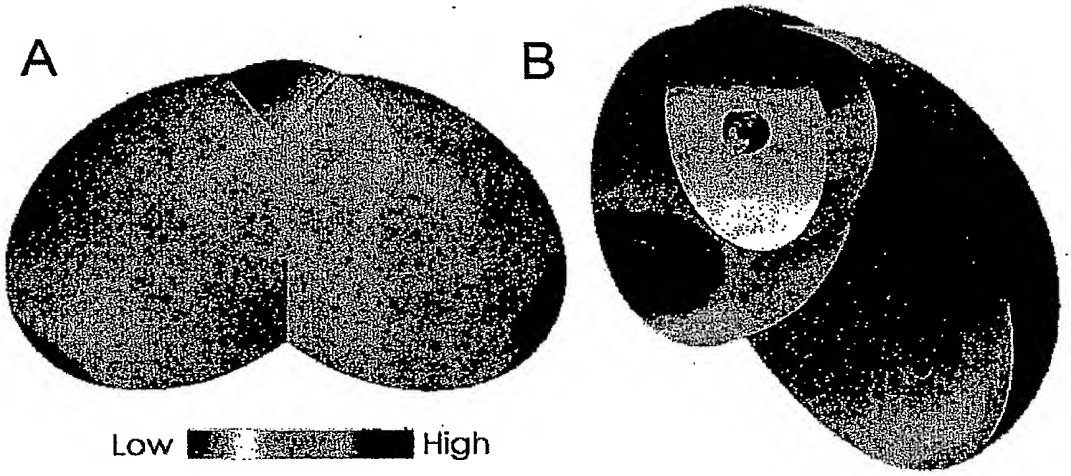


Fig.17

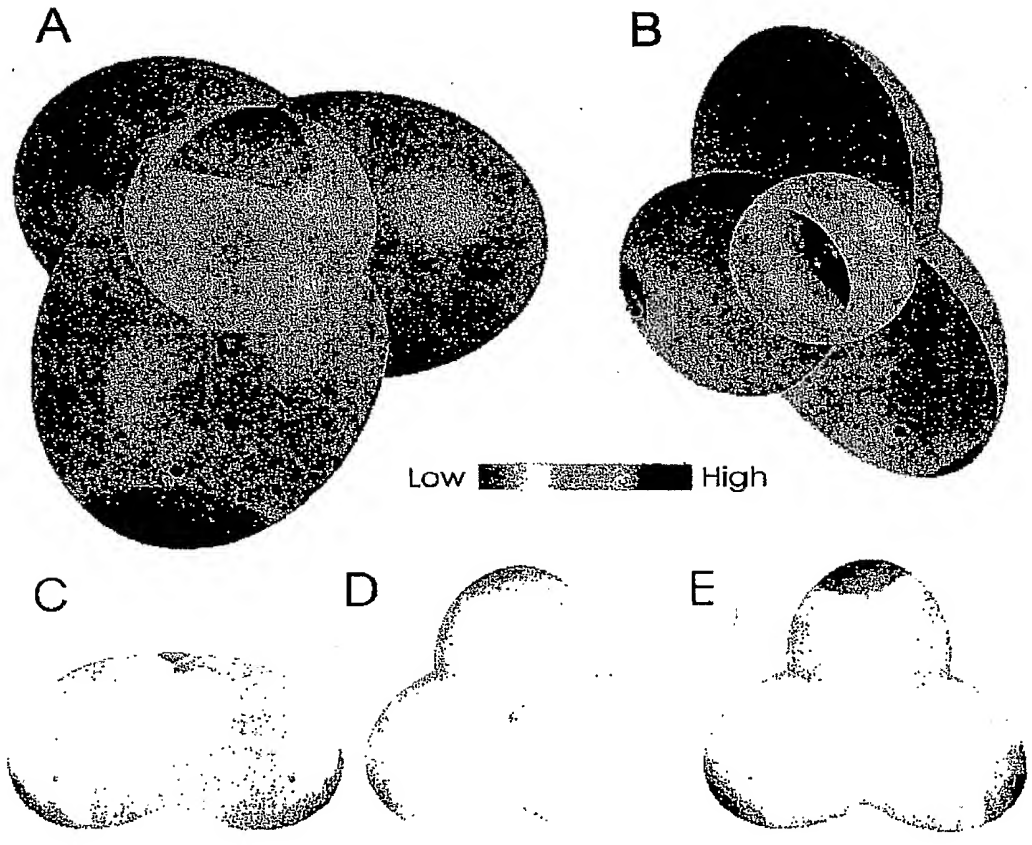


Fig.18

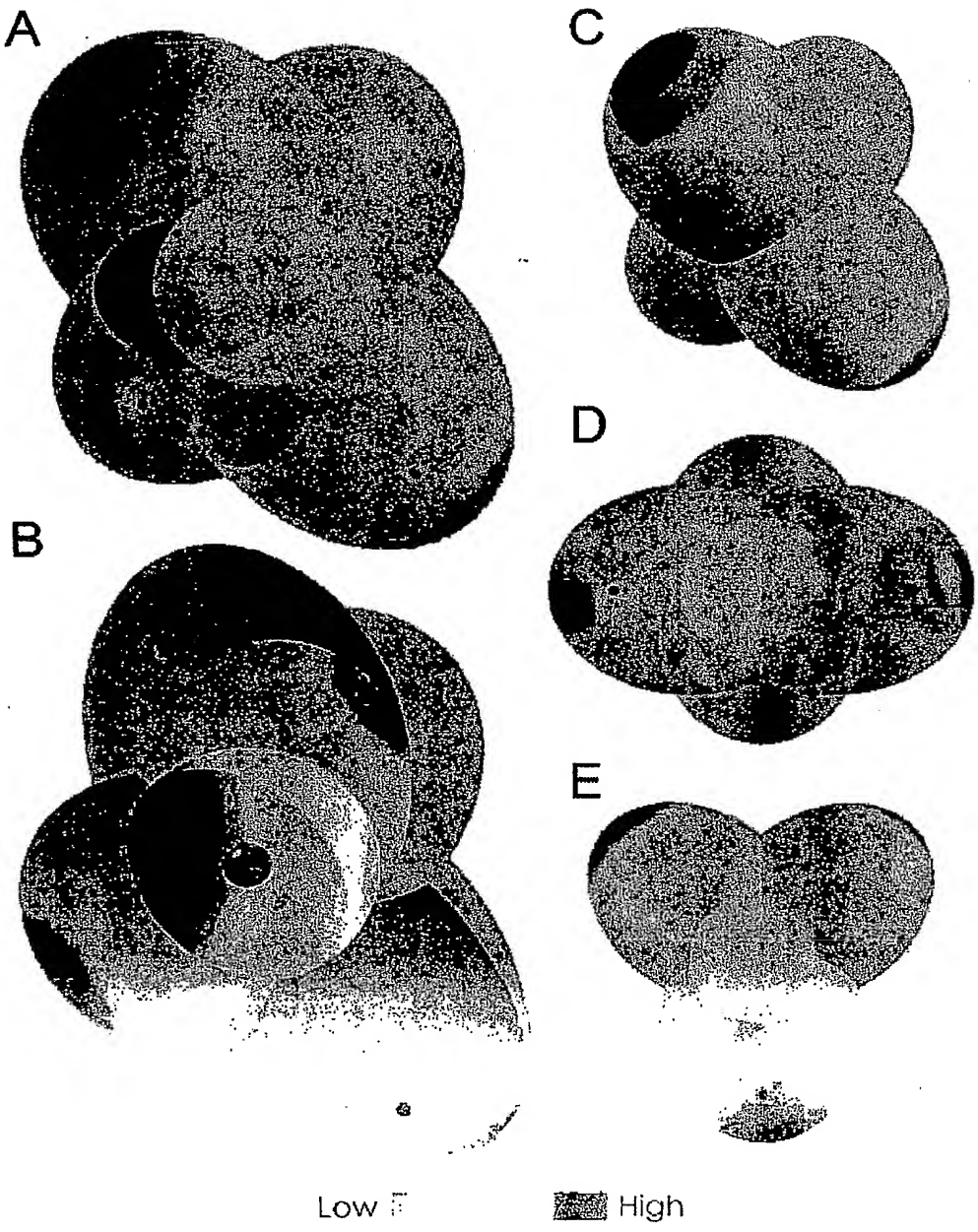


Fig.19

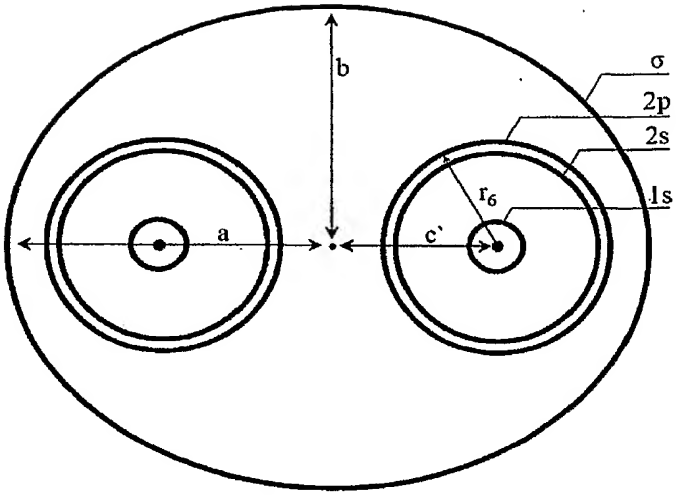


Fig.20

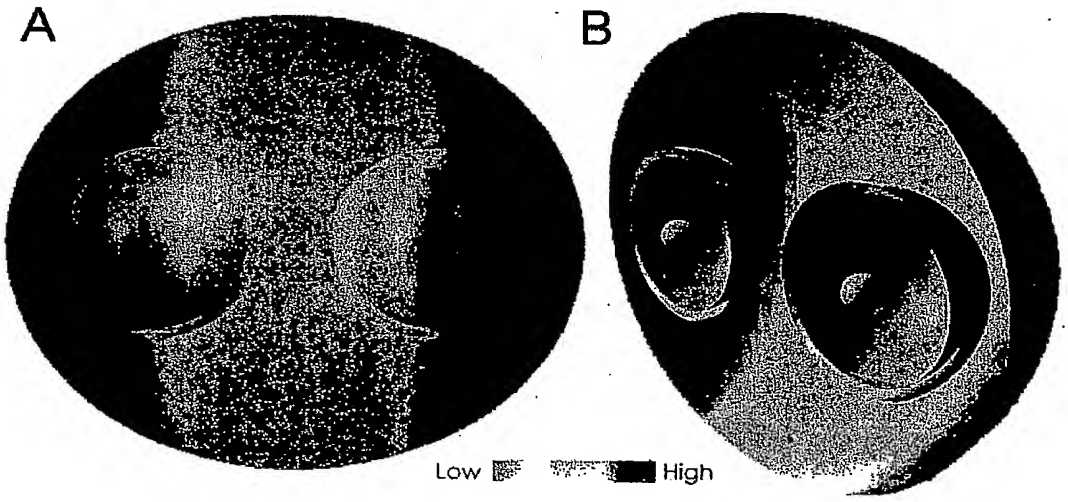


Fig.21

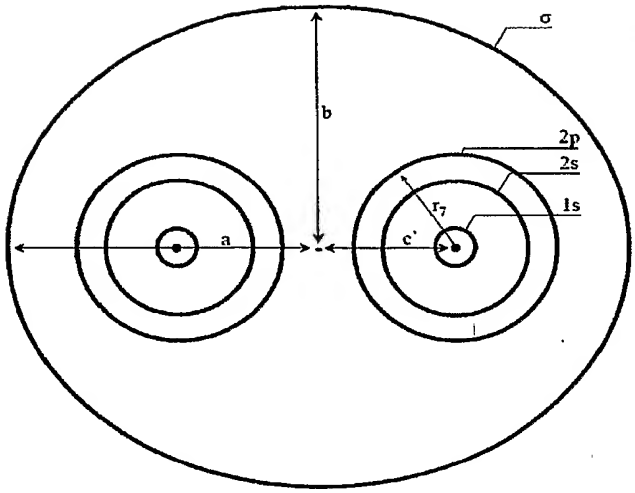


Fig.22

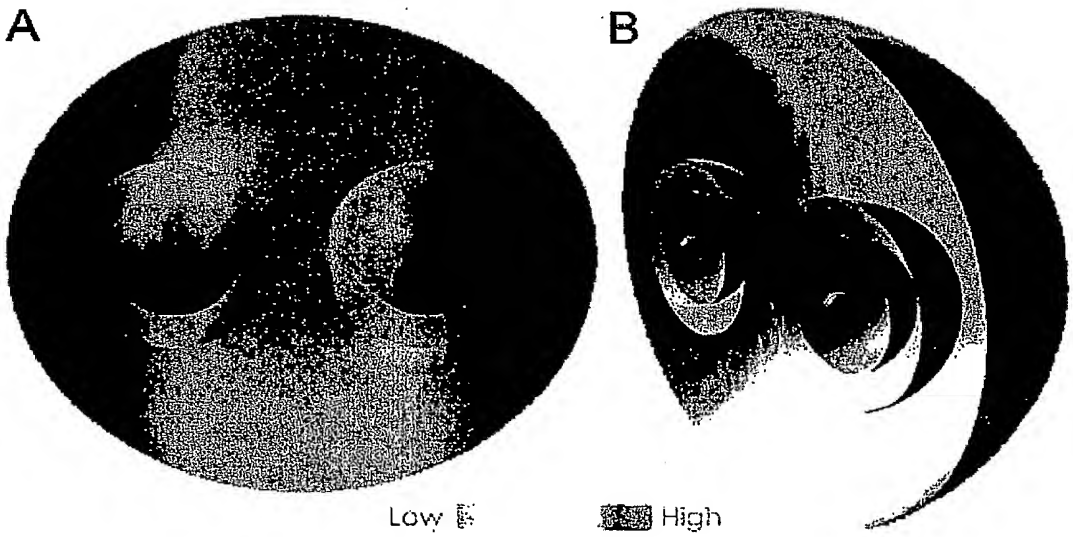


Fig.23

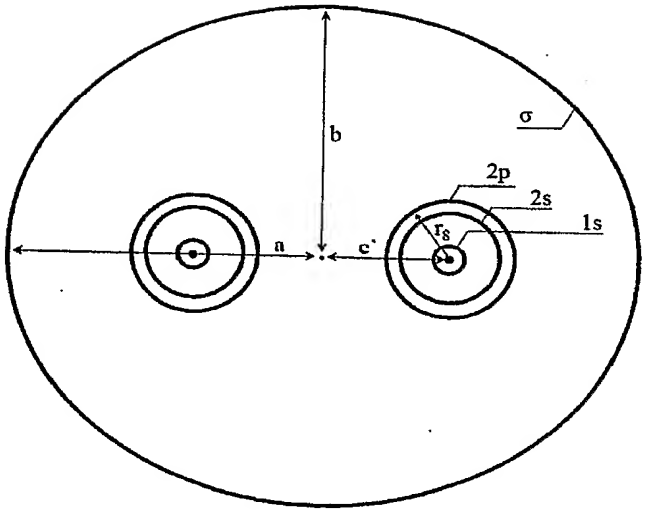


Fig.24

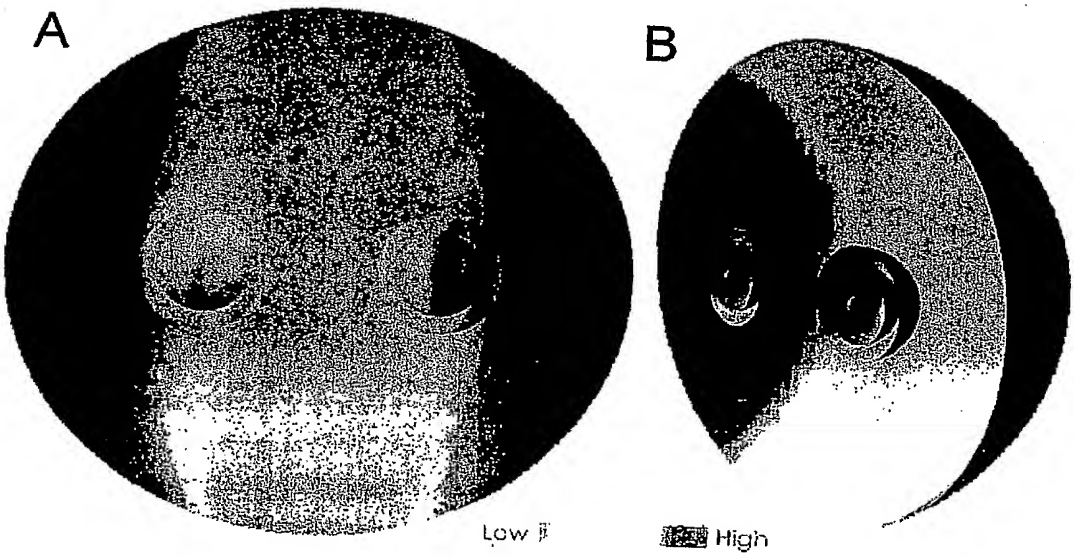


Fig.25

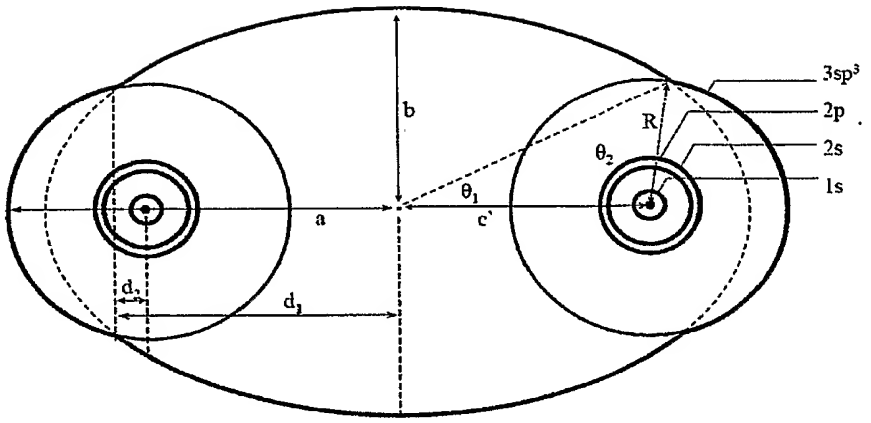


Fig.26

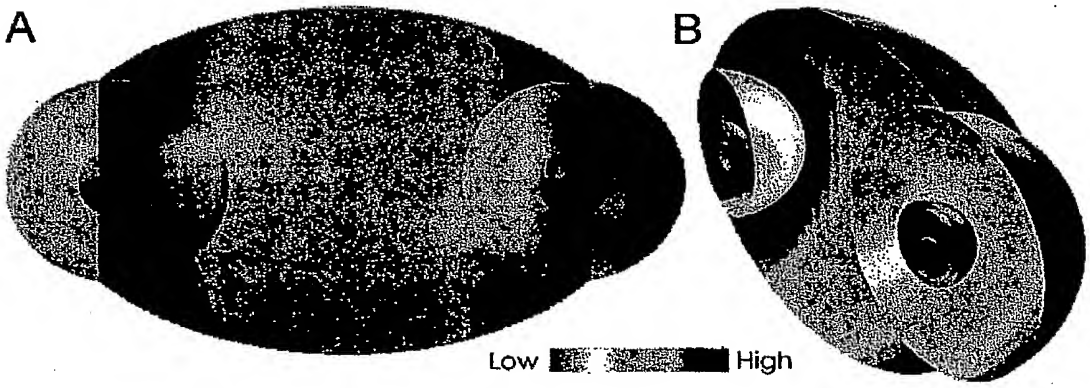


Fig.27

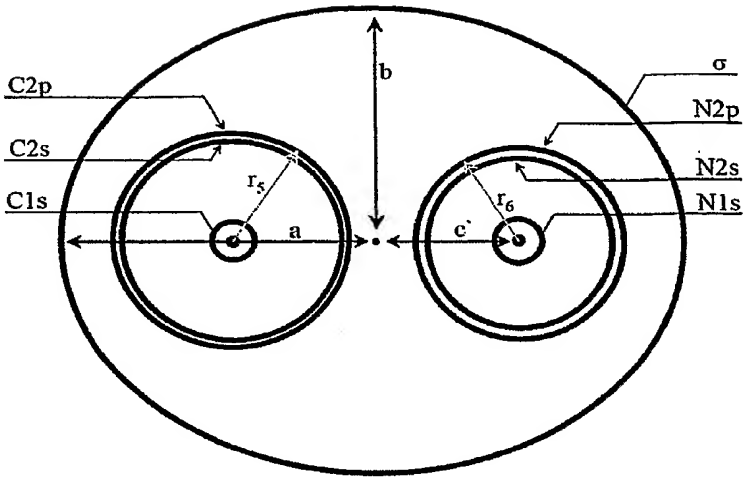


Fig.28

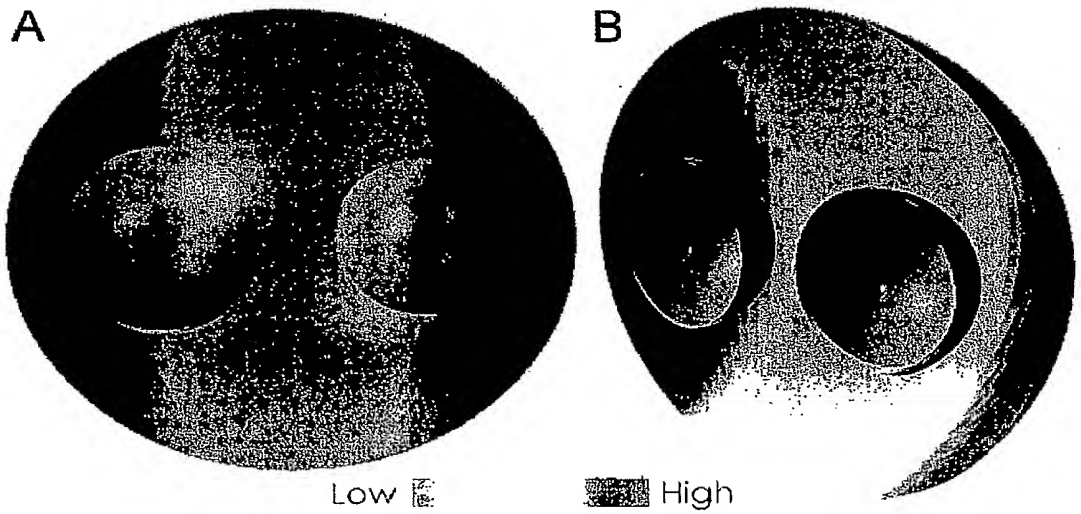


Fig.29

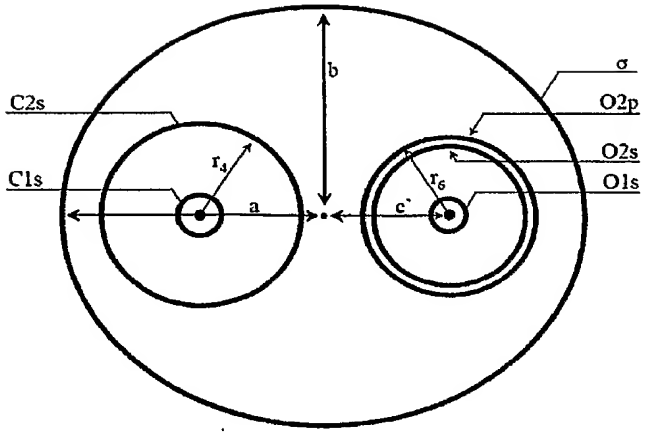


Fig.30

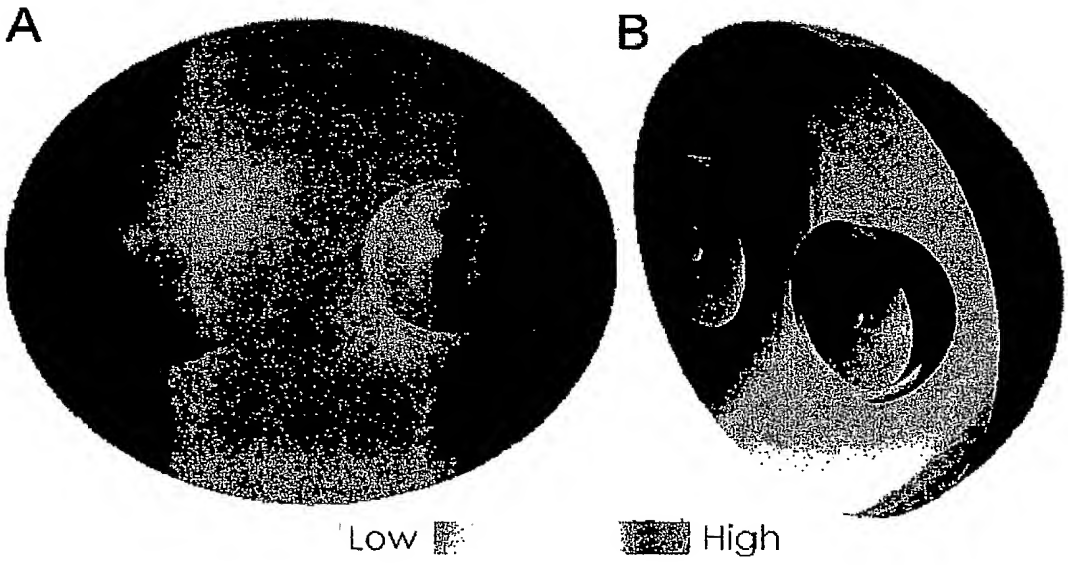


Fig.31

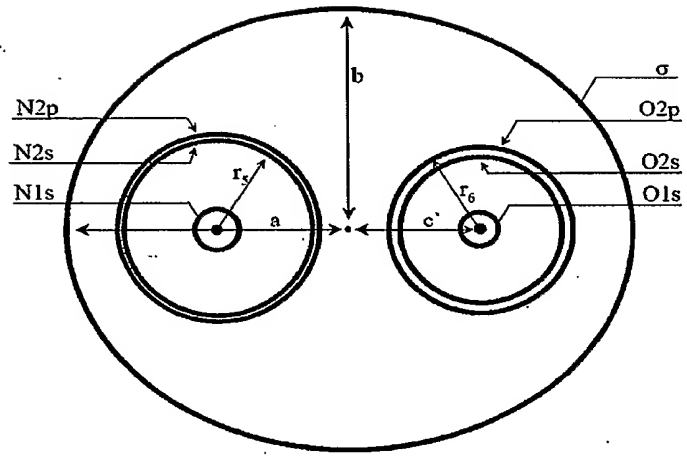


Fig.32

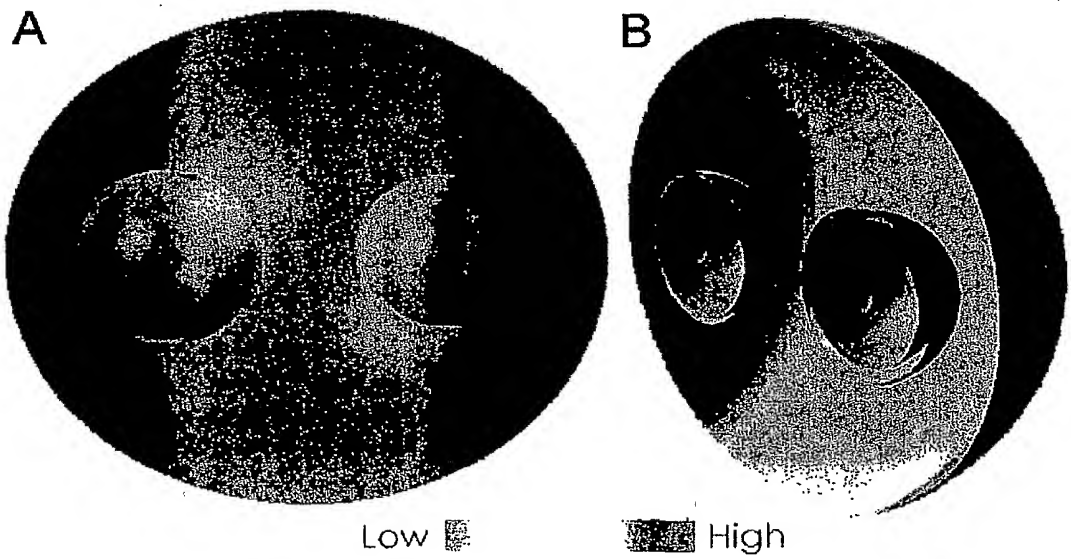


Fig.33

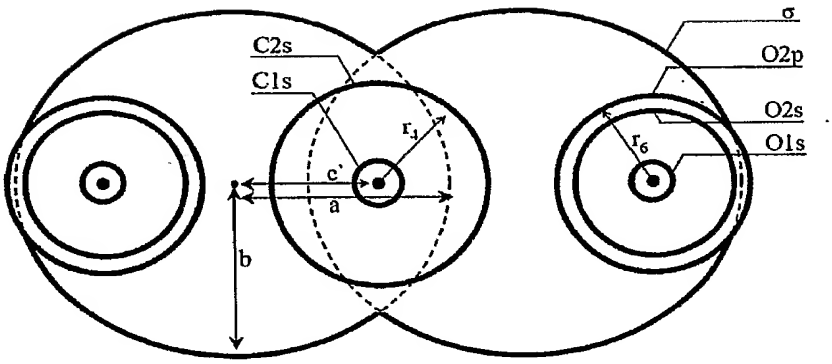
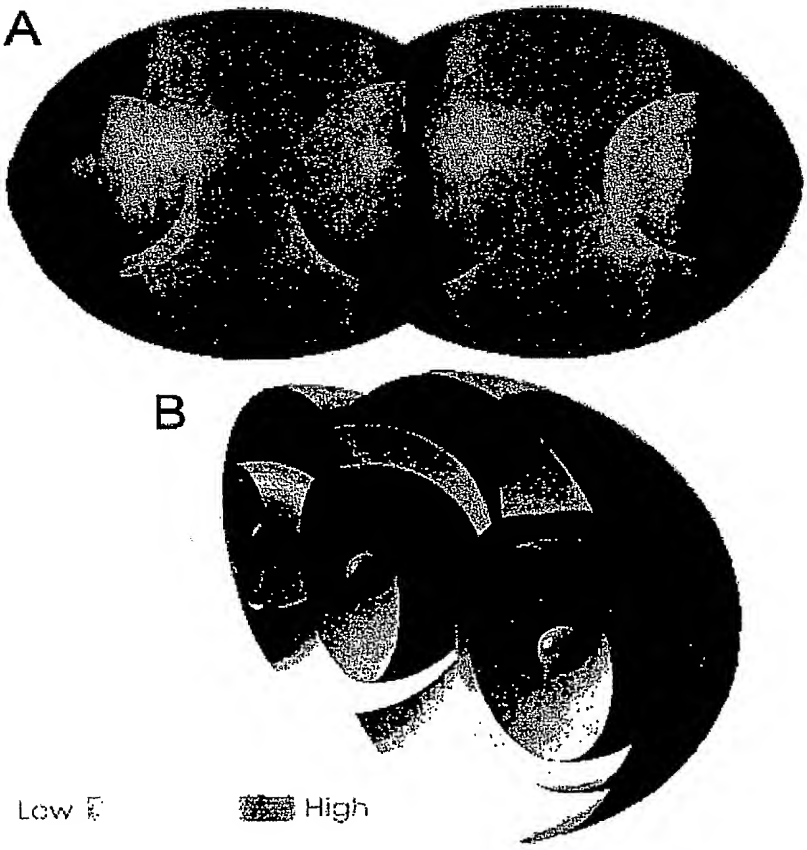


Fig.34



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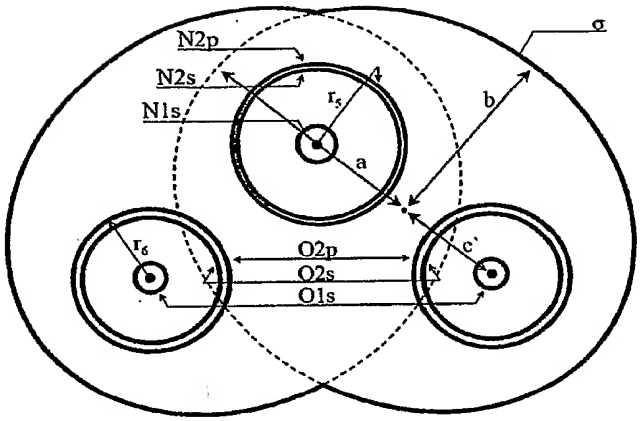


Fig.36

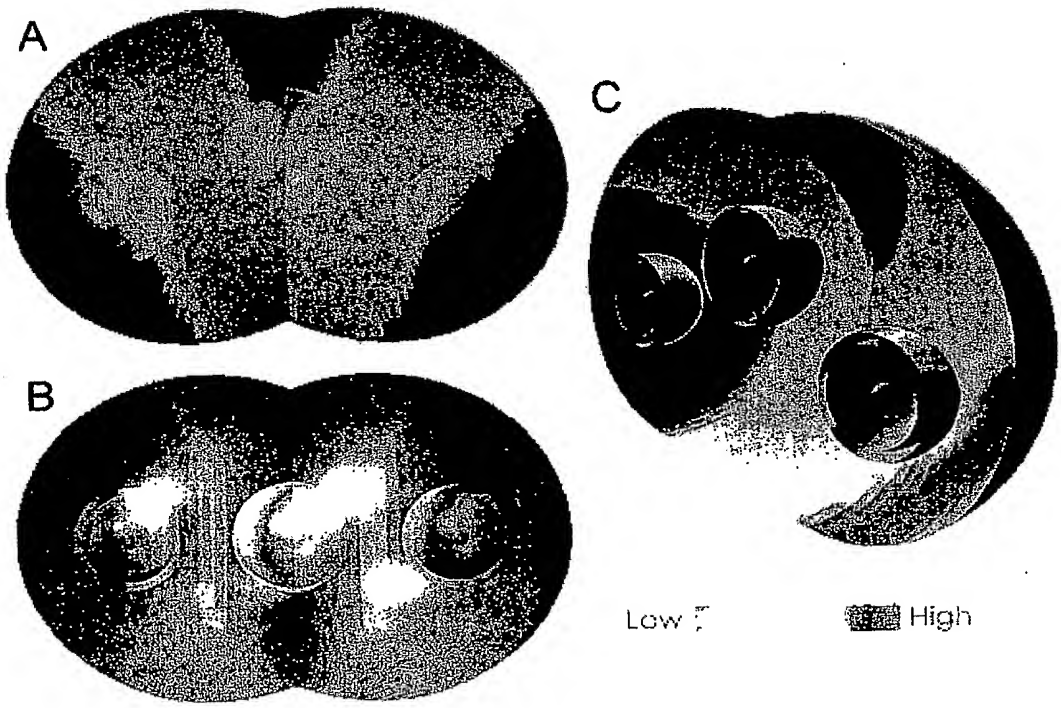


Fig.37

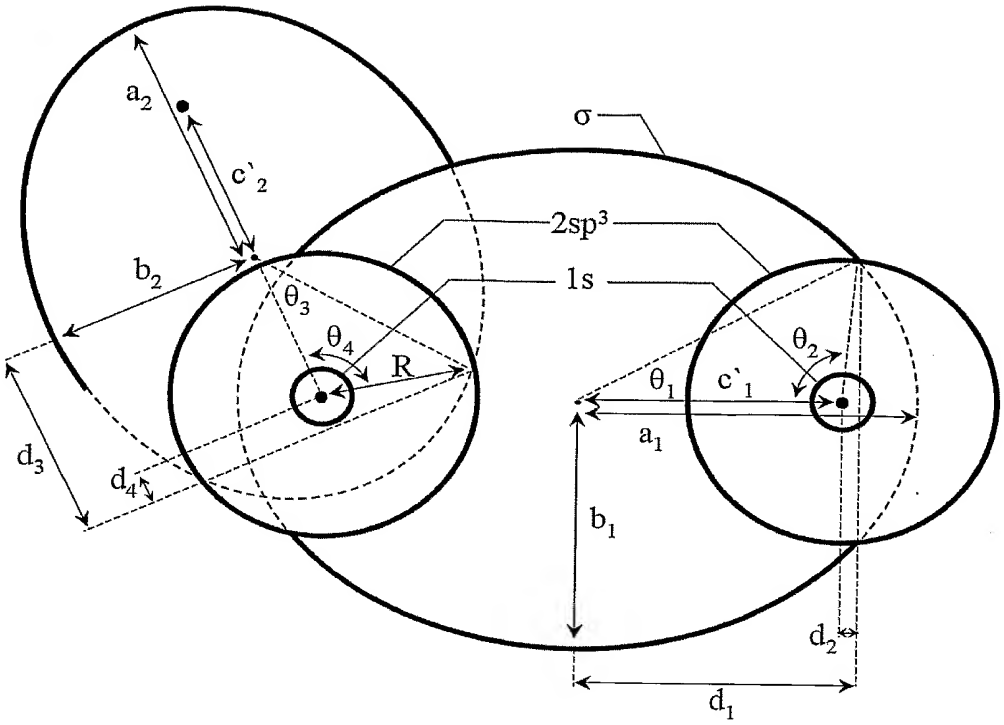

a2
c`2
σ
2sp3
b2
1s
θ3
θ4
R
θ2
θ1
c`1
a1
d3
d4
b1
d2
d1

Fig.38

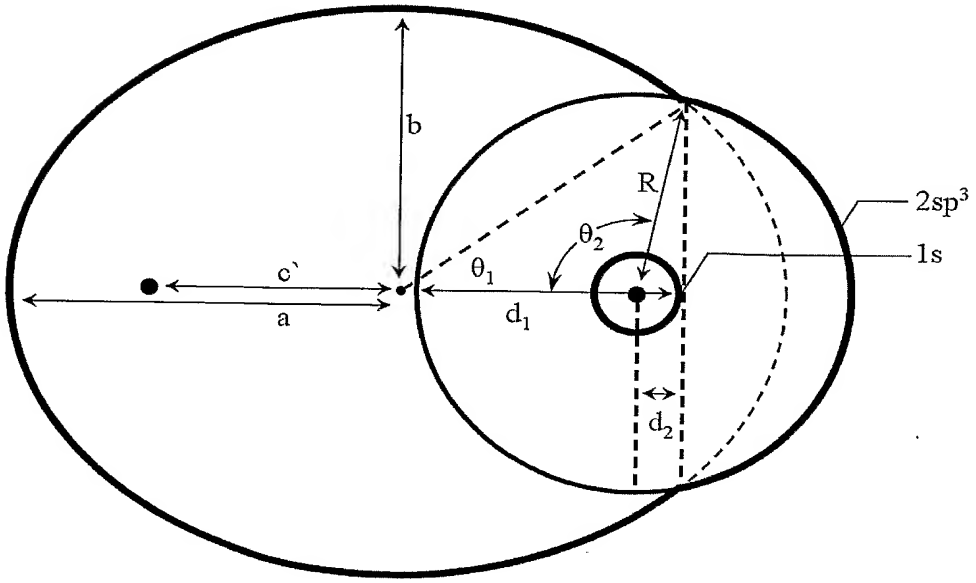

b
R
2sp3
θ2
1s
c`
θ1
a
d1
d2

Fig.39

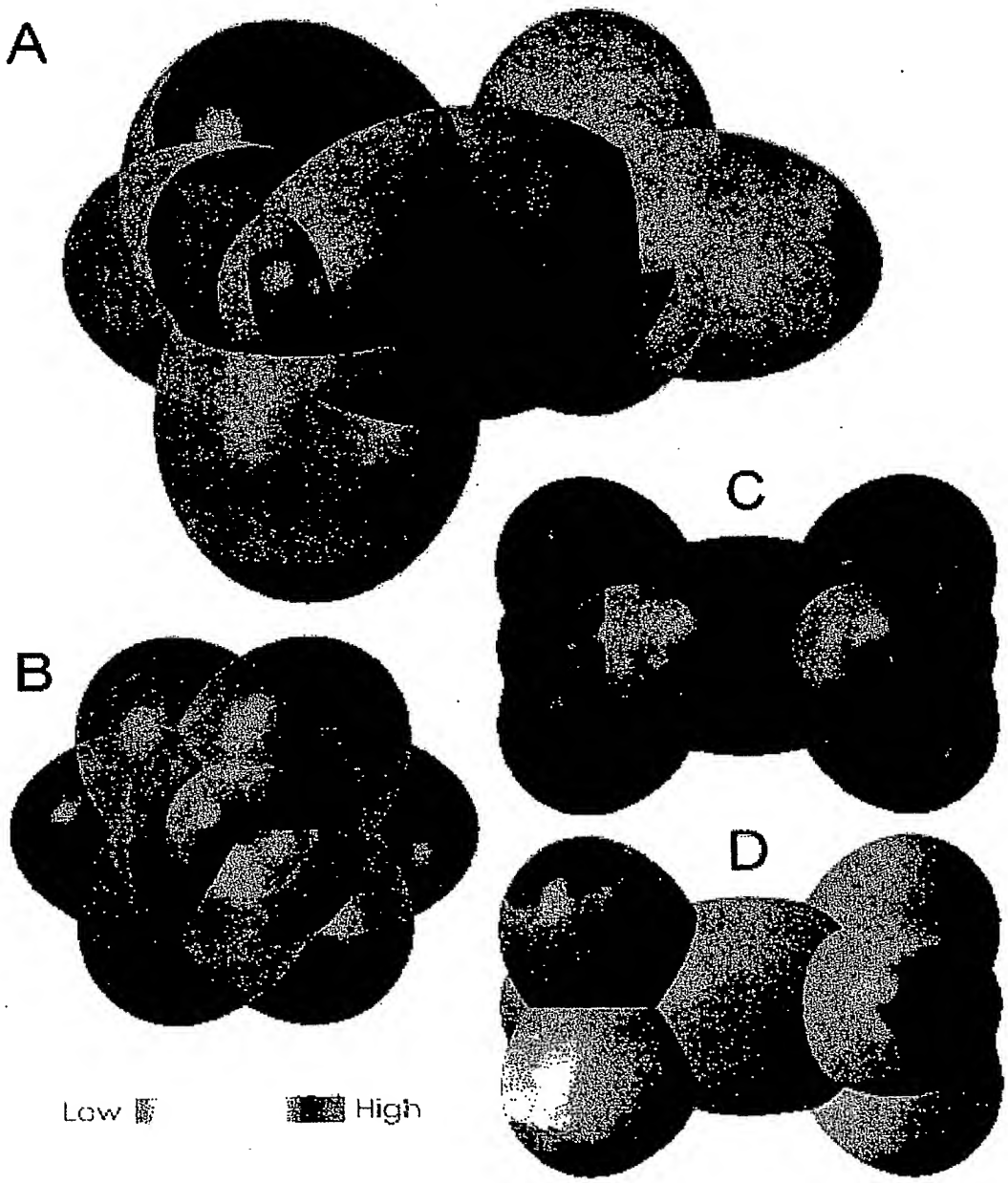


Fig.40

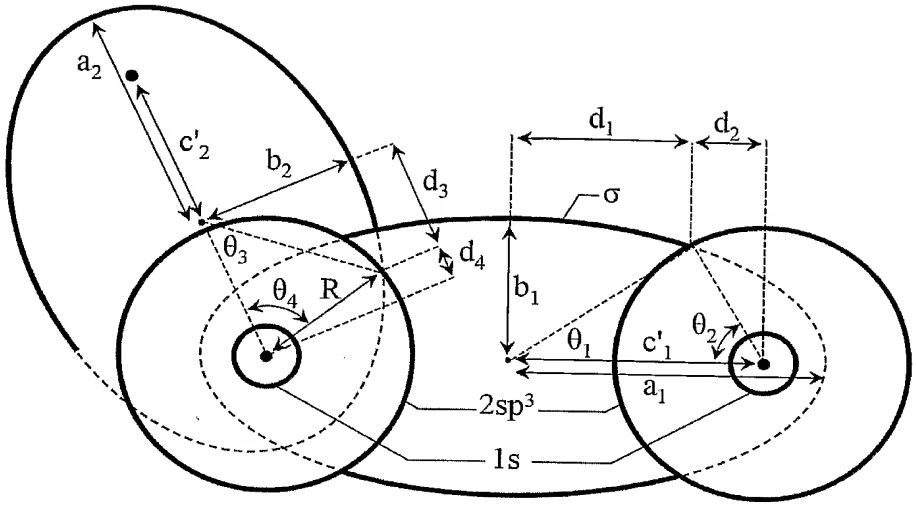

a2
c'2
b2
d3
d1
d2
σ
θ3
d4
θ4
R
b1
θ1
c'1
θ2
a1
2sp3
1s

Fig.41

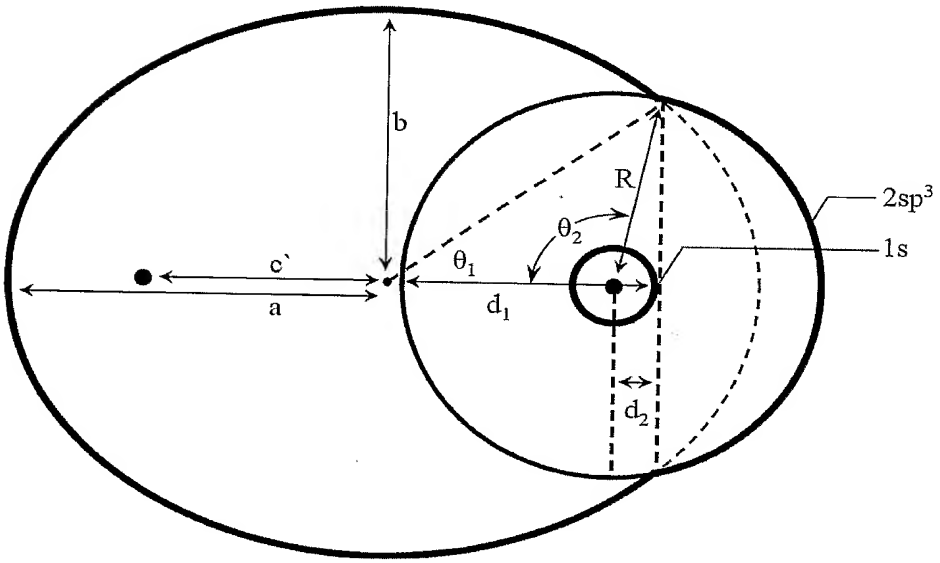

b
R
2sp3
θ2
1s
c`
θ1
a
d1
d2

Fig.42

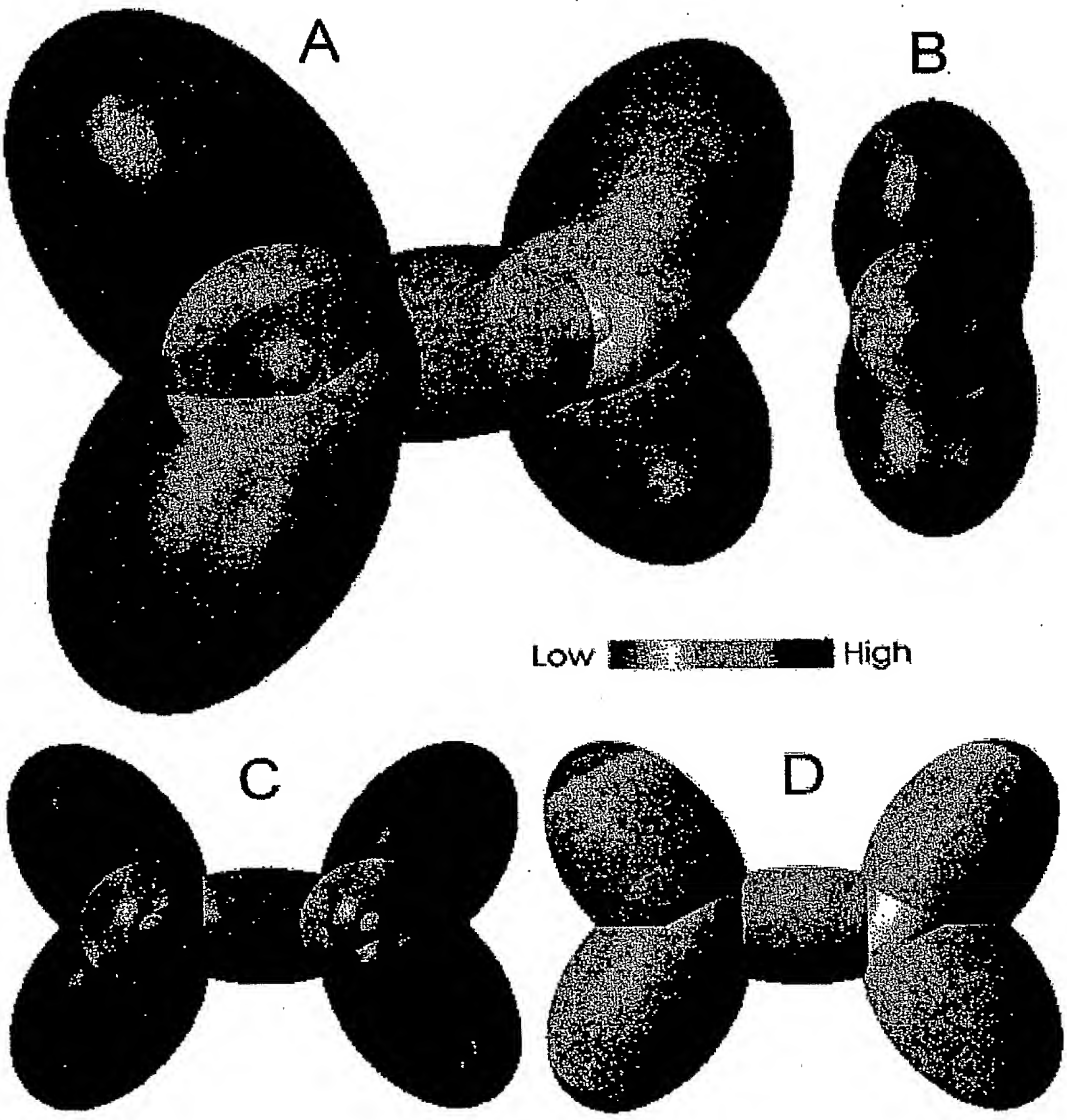


Fig.43

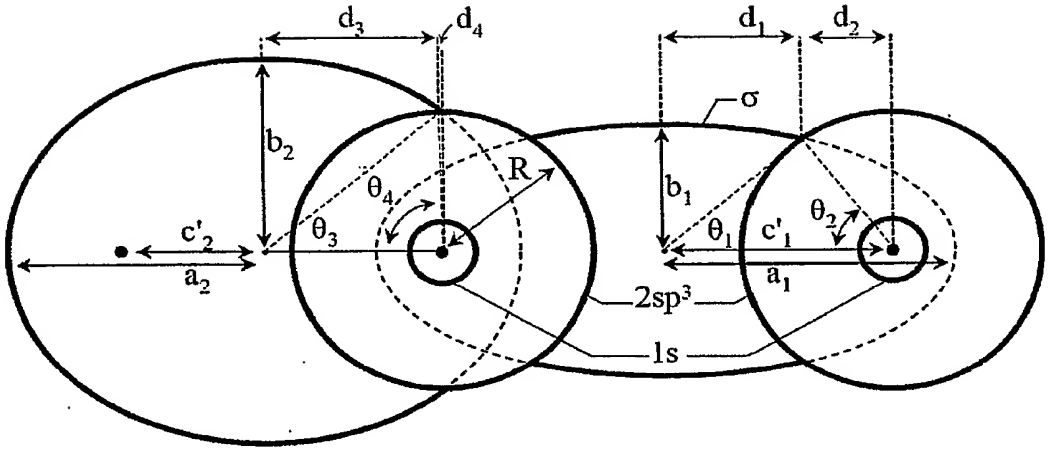


Fig.44

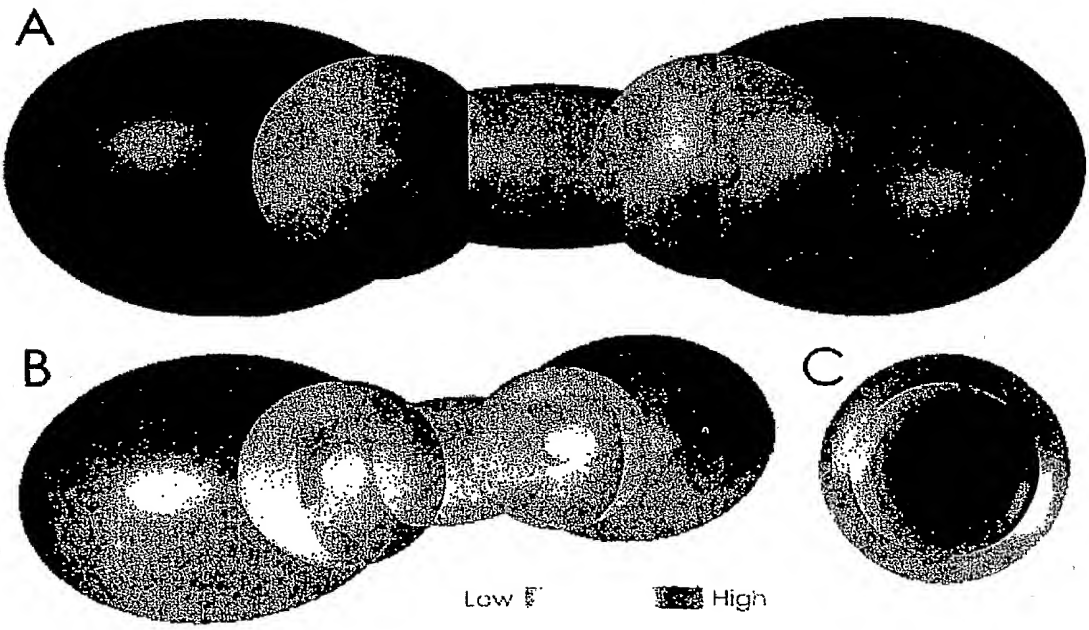


Fig.45

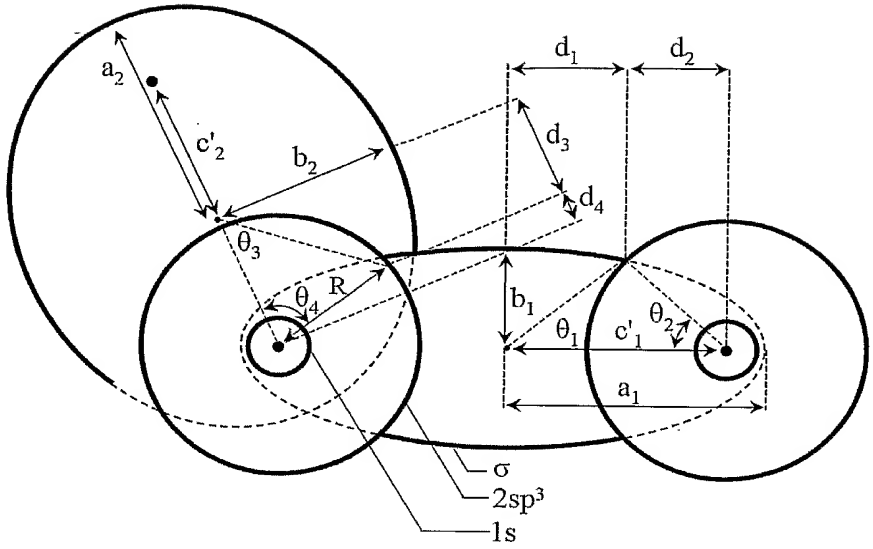

a2
c'2
b2
θ3
θ4
R
d1
d2
d3
d4
b1
θ1
c'1
θ2
a1
σ
2sp3
1s

Fig.46

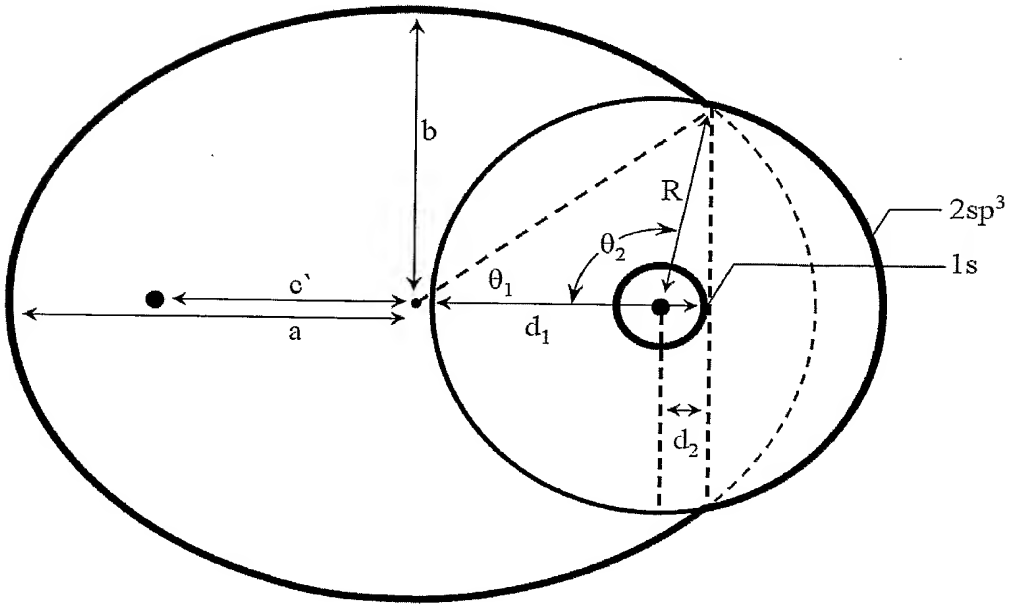
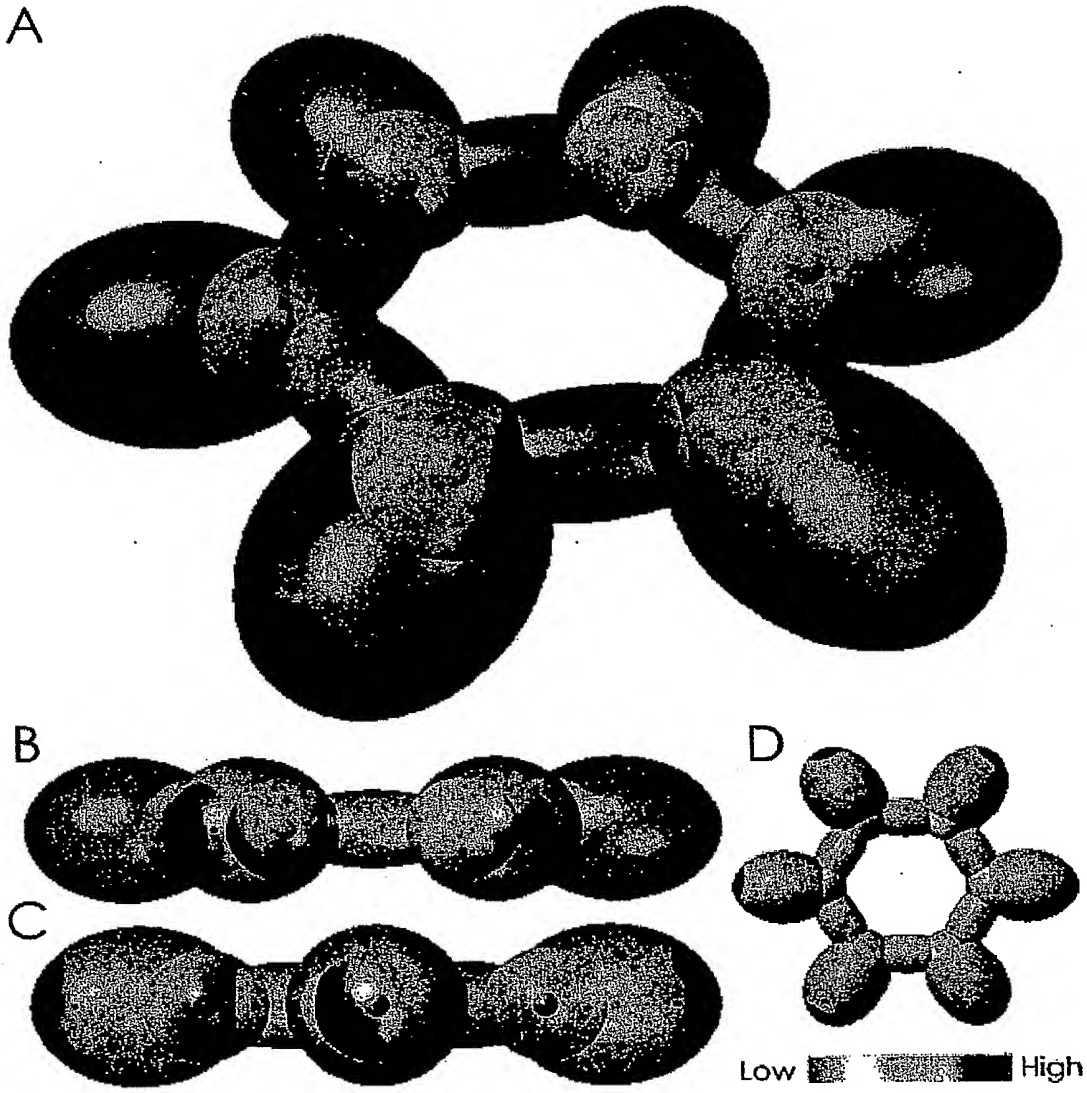

b
c'
a
θ1
θ2
R
d1
d2
2sp3
1s

Fig.47



28/51
Fig.48

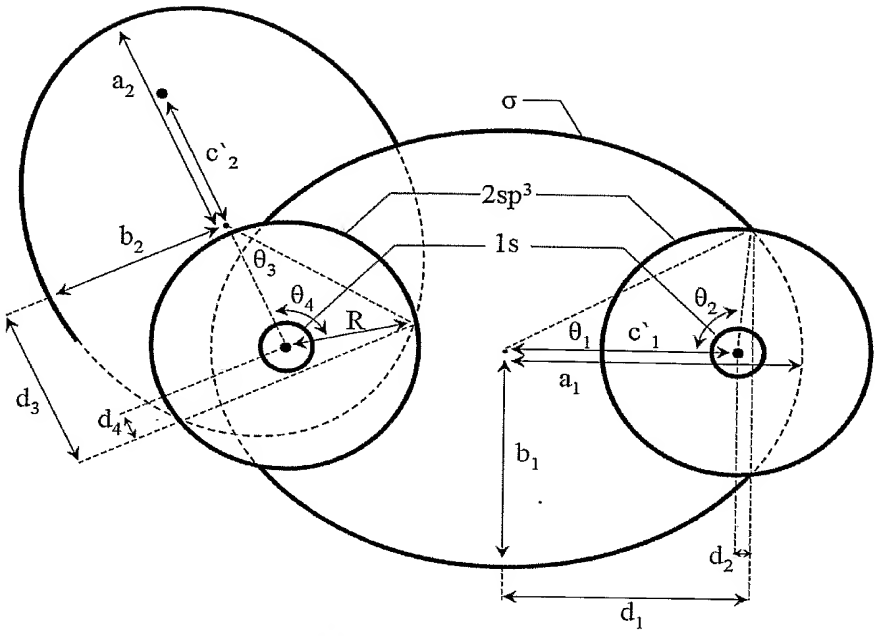


Fig.49

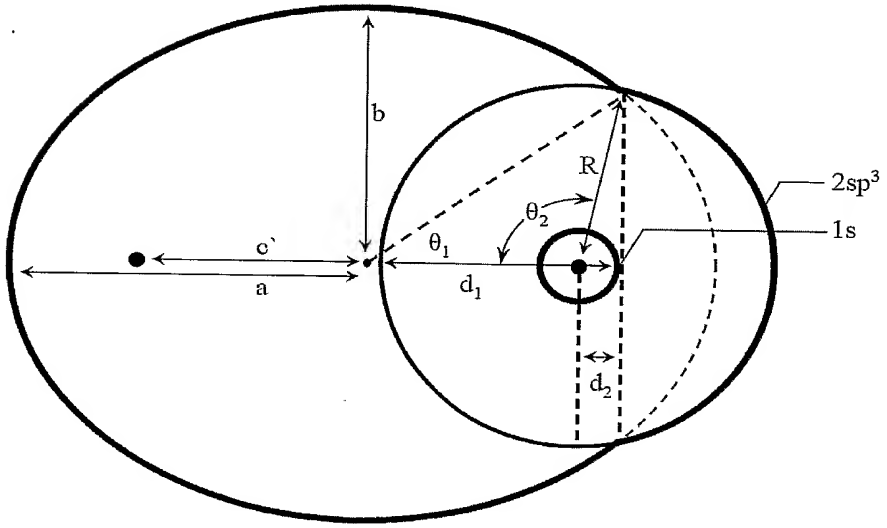


Fig.50

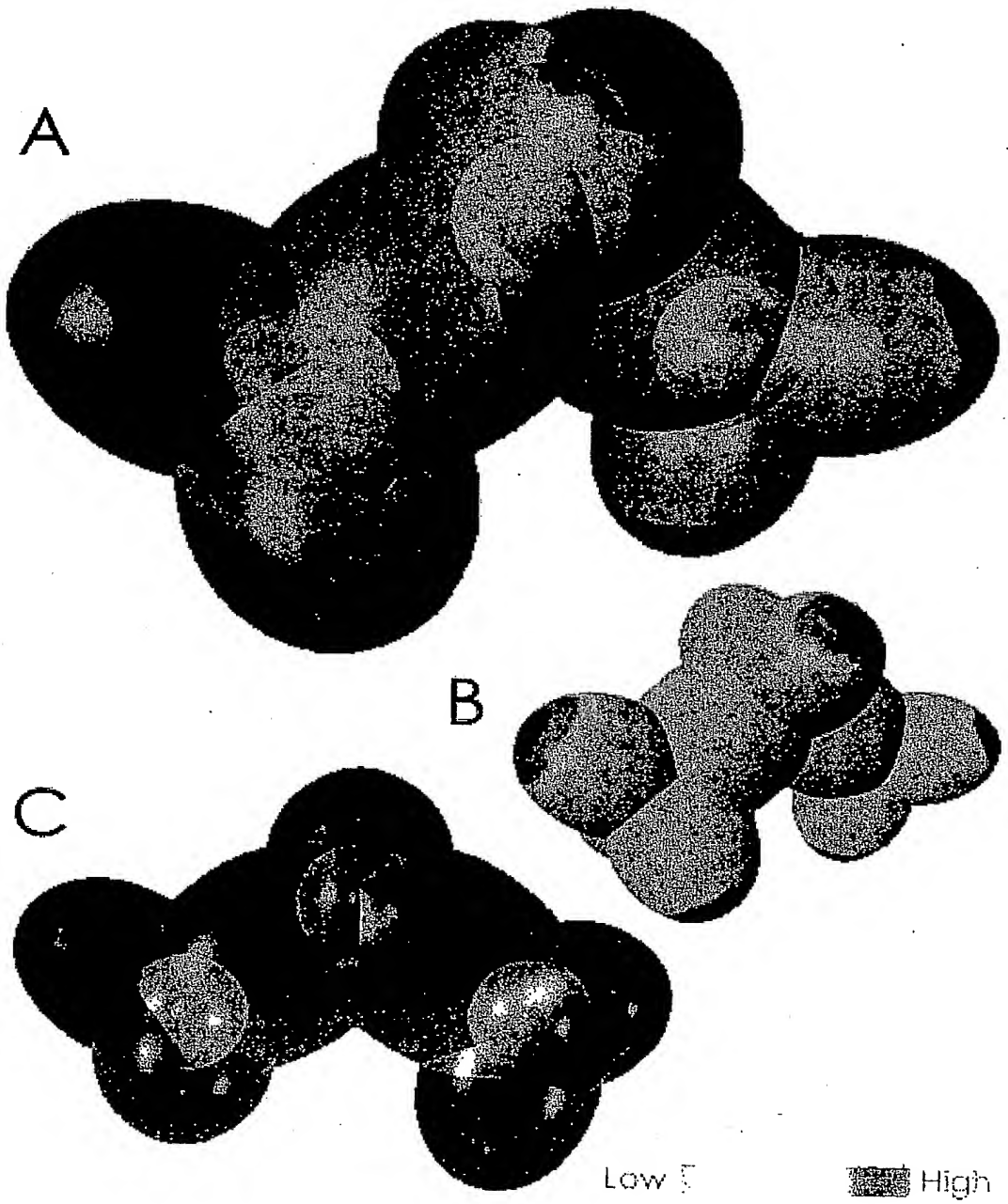


Fig.51

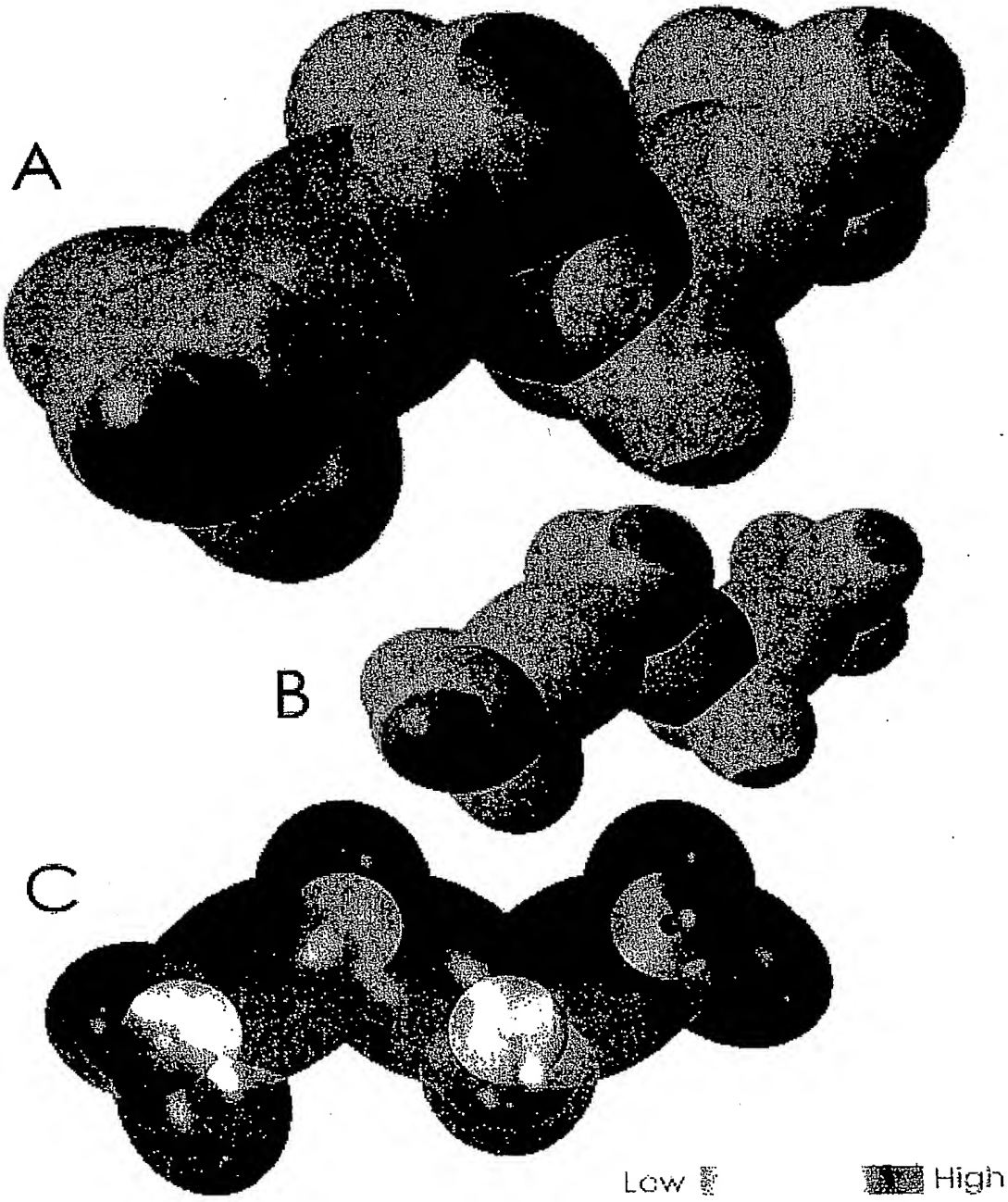


Fig.52

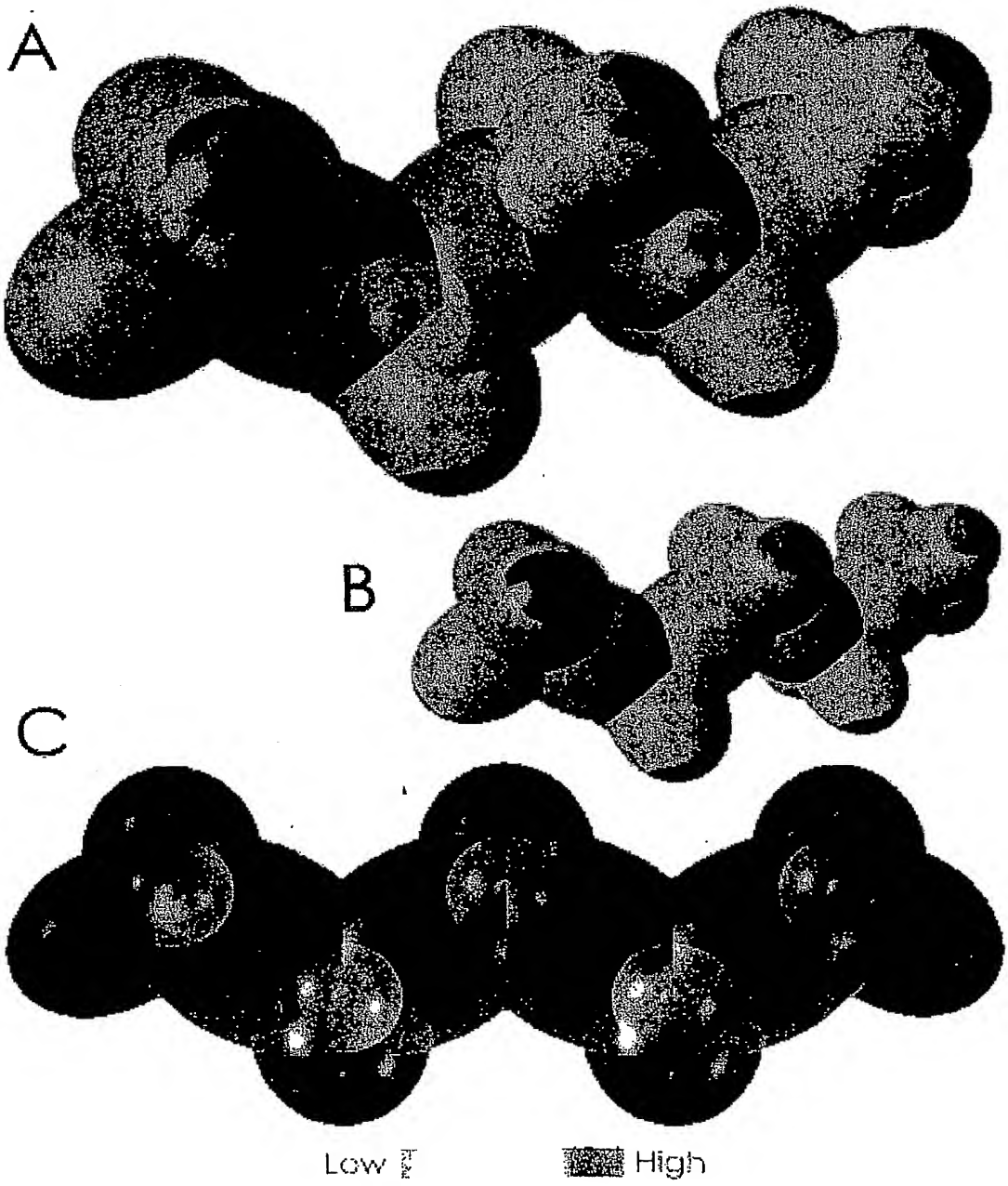


Fig.53

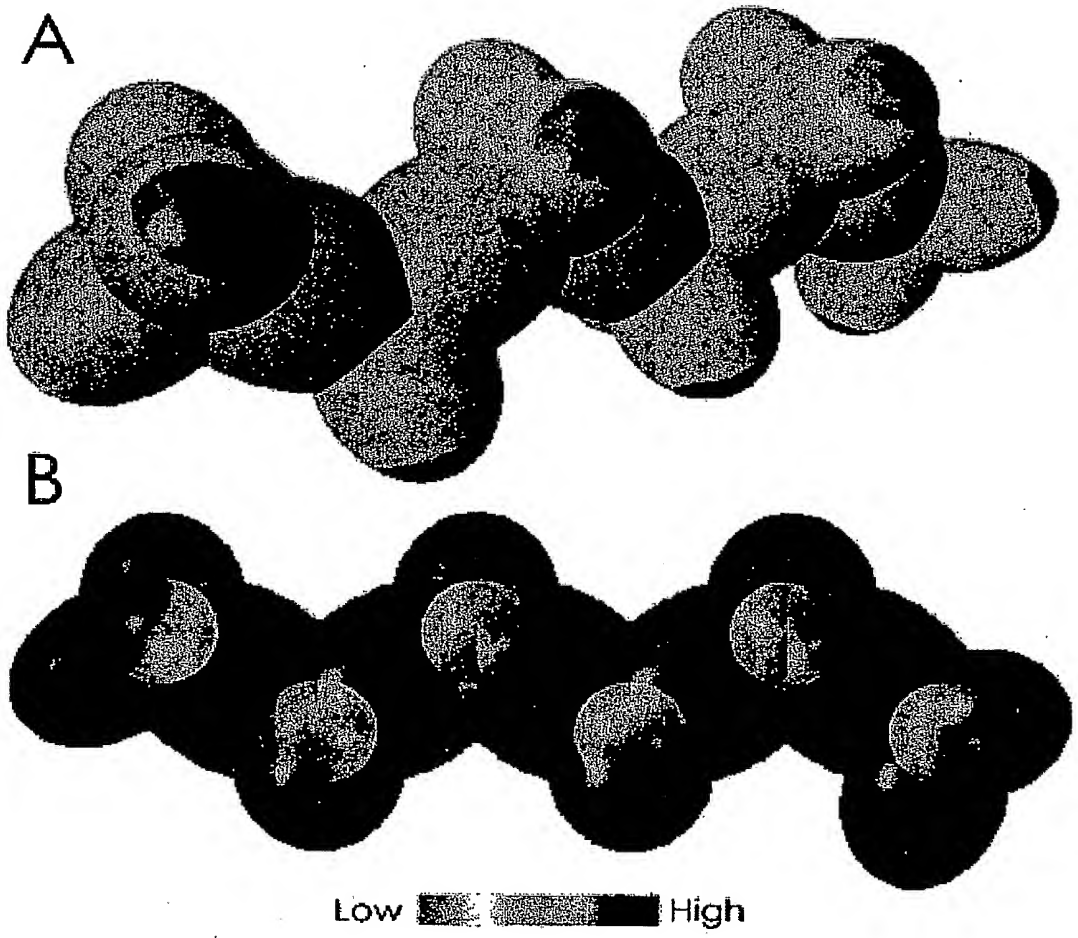


Fig.54

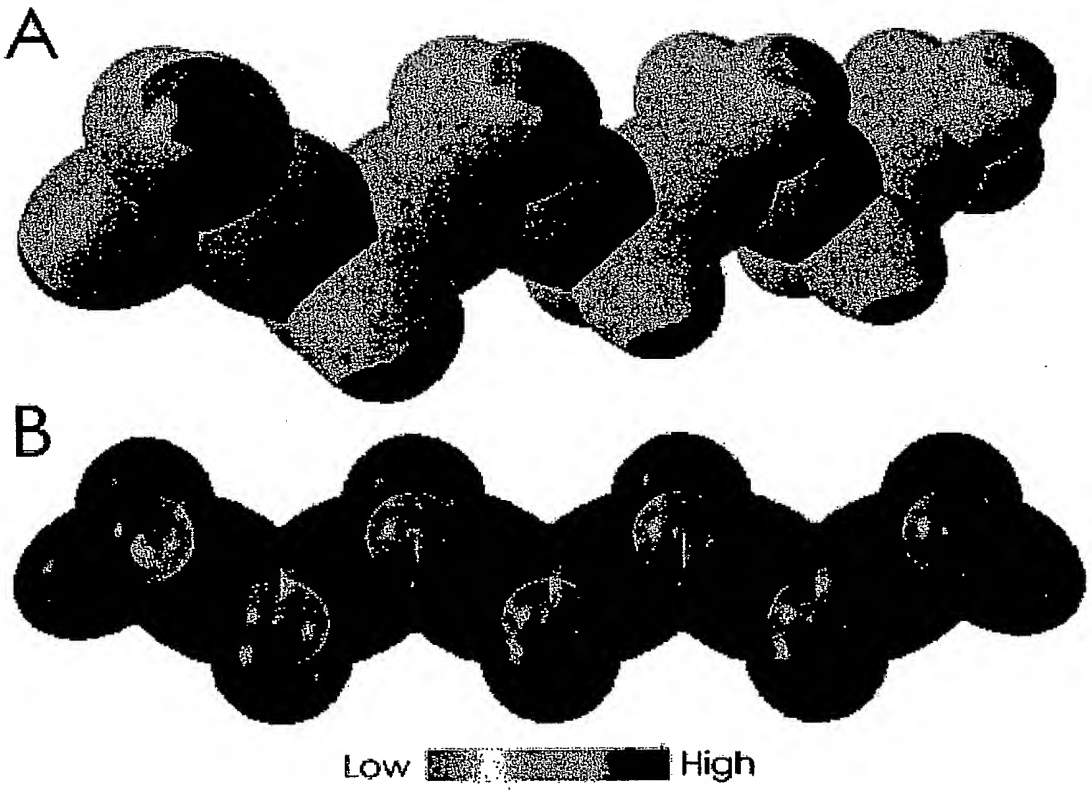


Fig.55

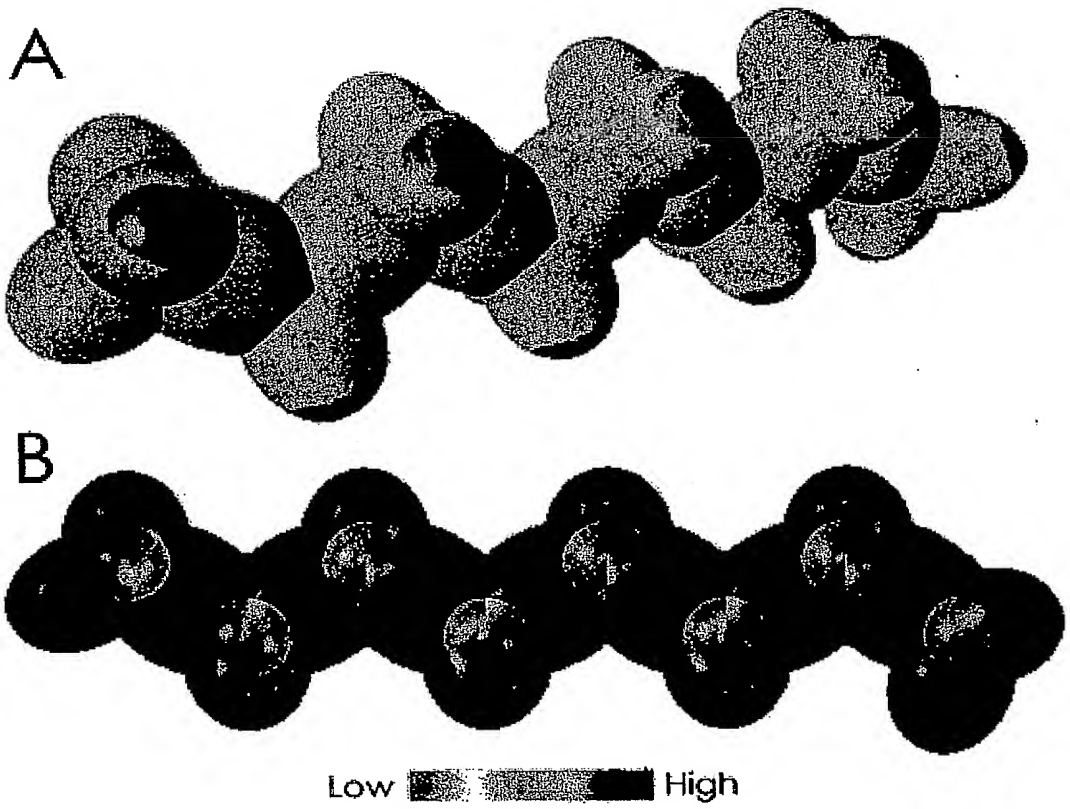


Fig.56

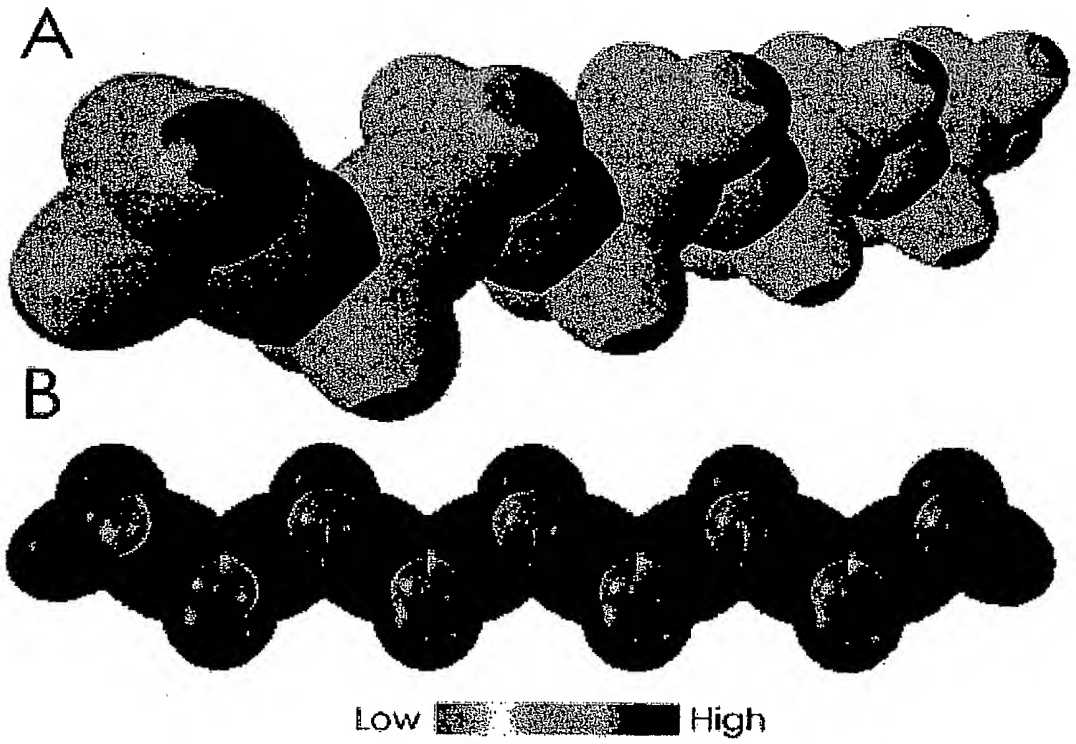


Fig.57

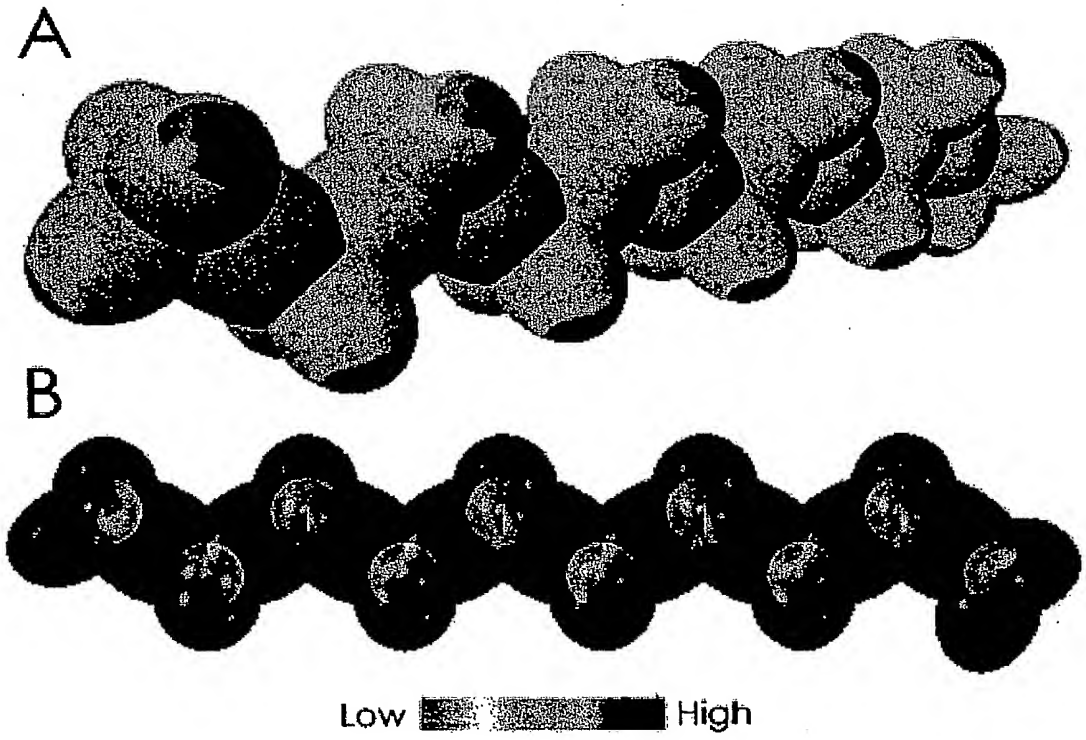


Fig.58

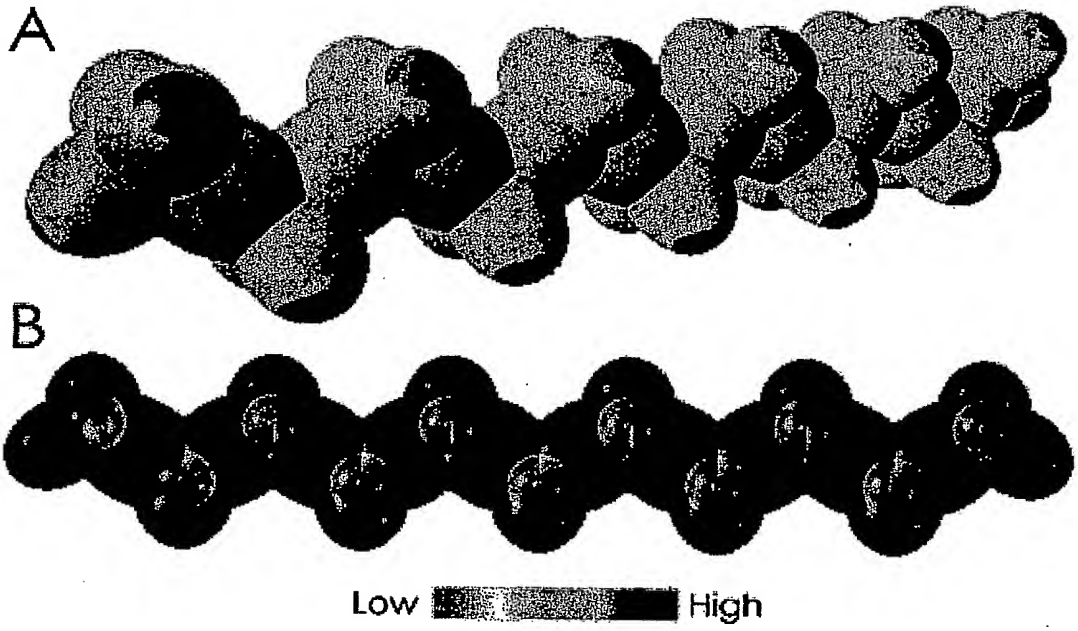


Fig.59

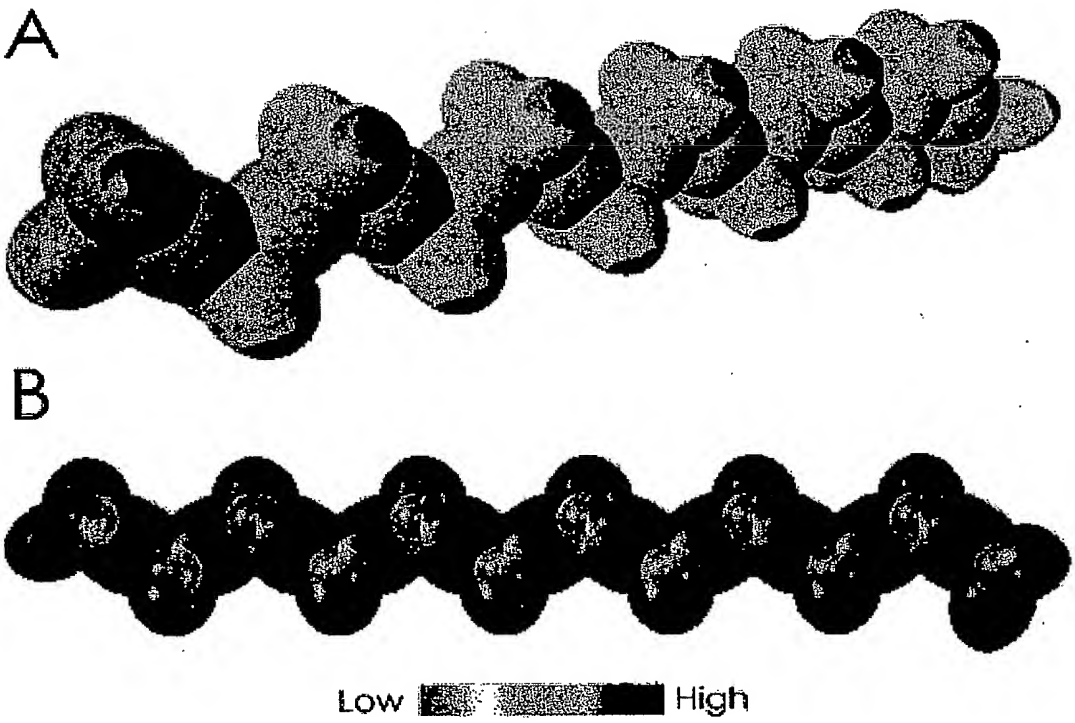


Fig.60

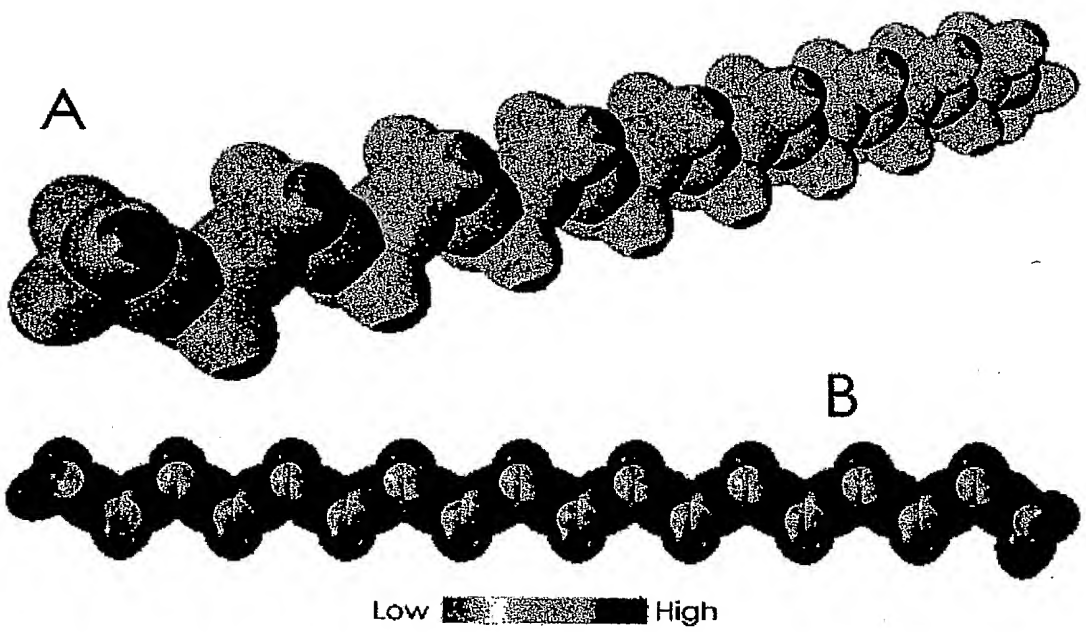


Fig. 61.A

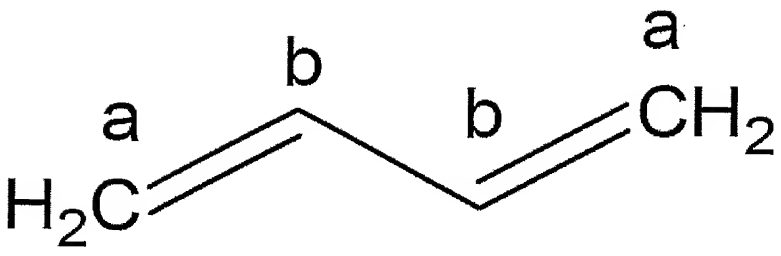


Fig. 61.B

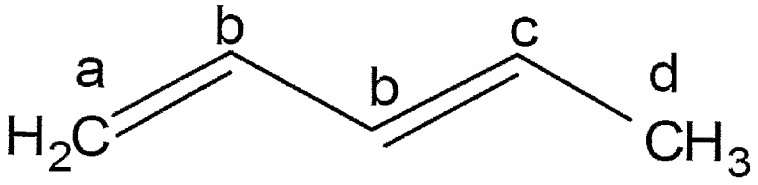


Fig. 61.C

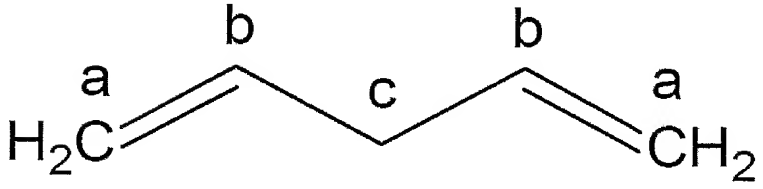


Fig. 61.D

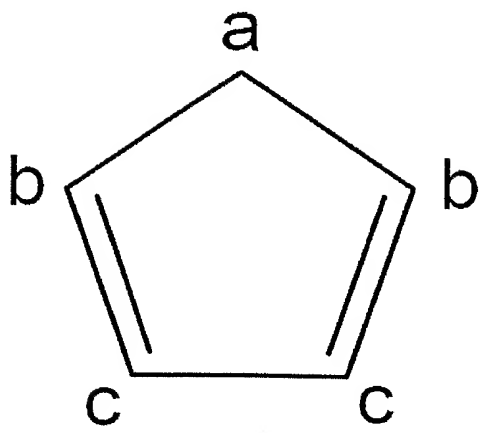


Fig. 61E

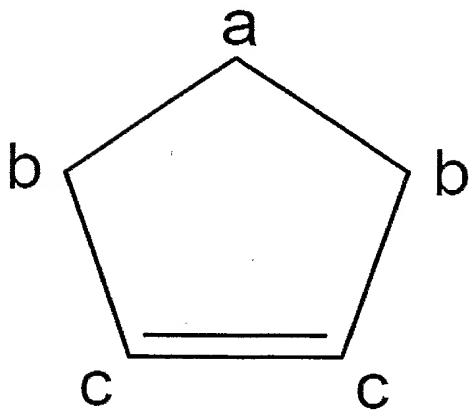


Fig. 62

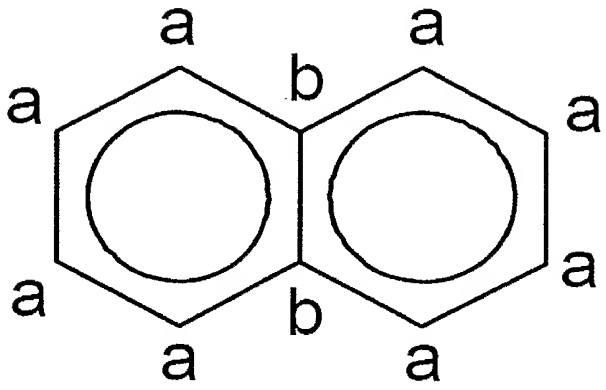


Fig. 63

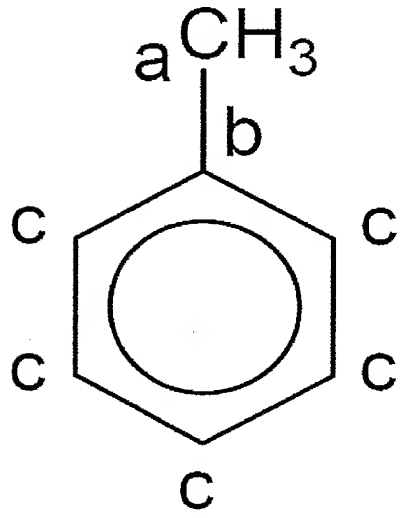


Fig. 64

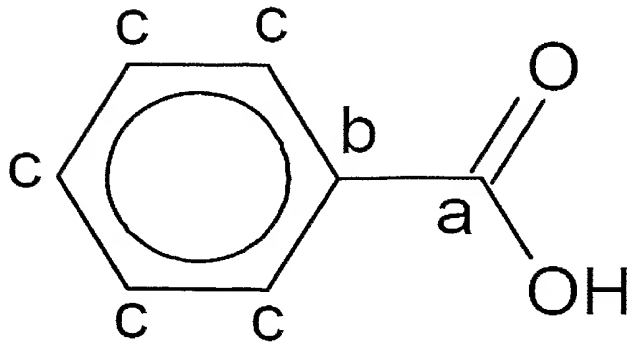
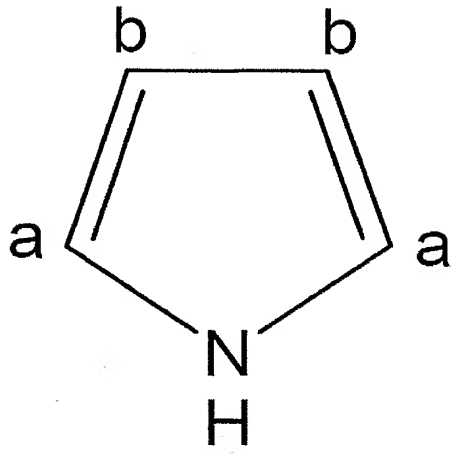


Fig. 65



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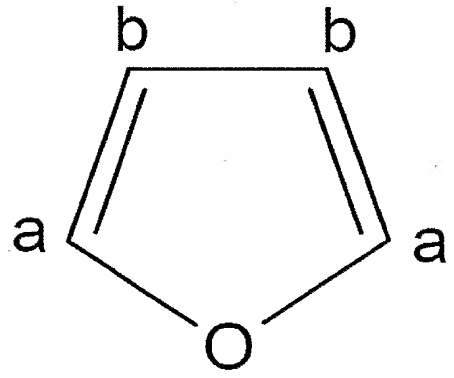
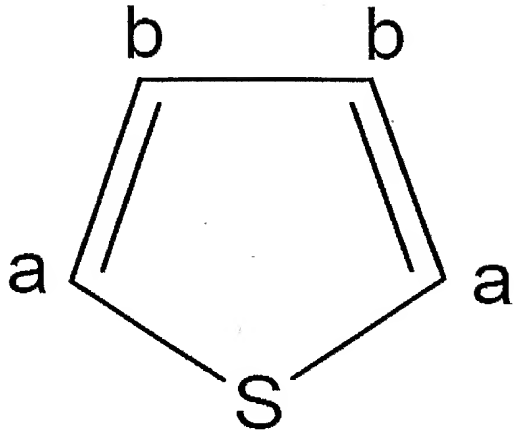


Fig. 67



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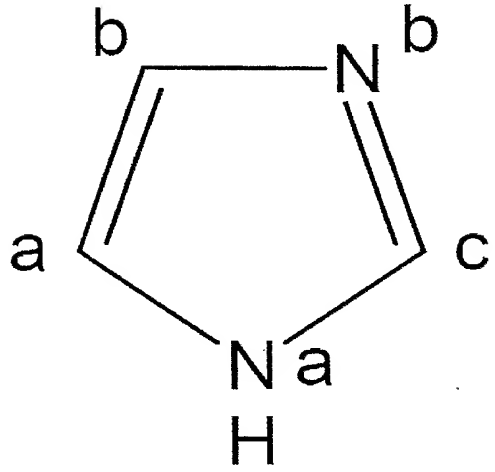

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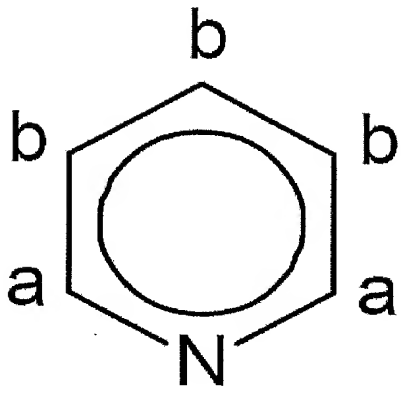


Fig. 70

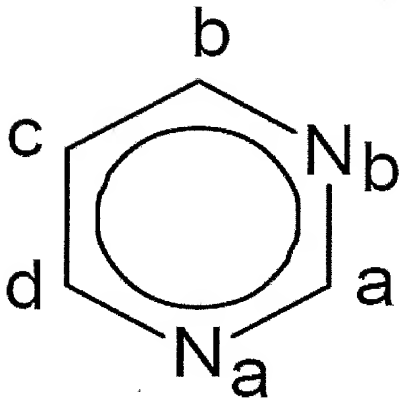


Fig. 71

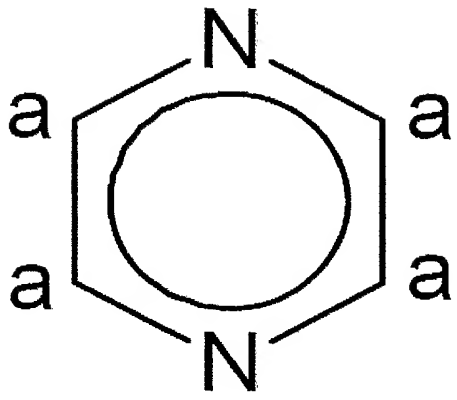


Fig.72

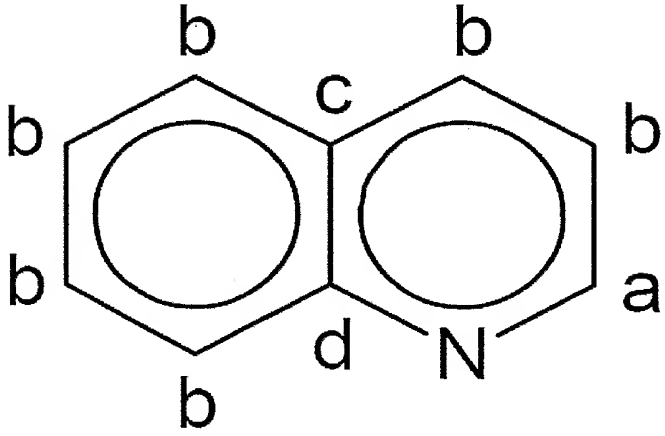


Fig. 73

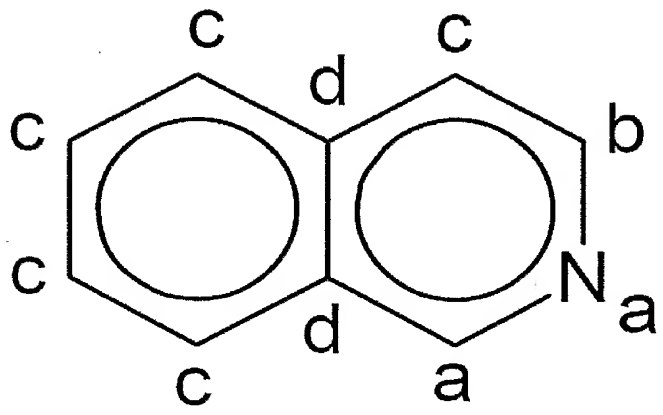


Fig. 74

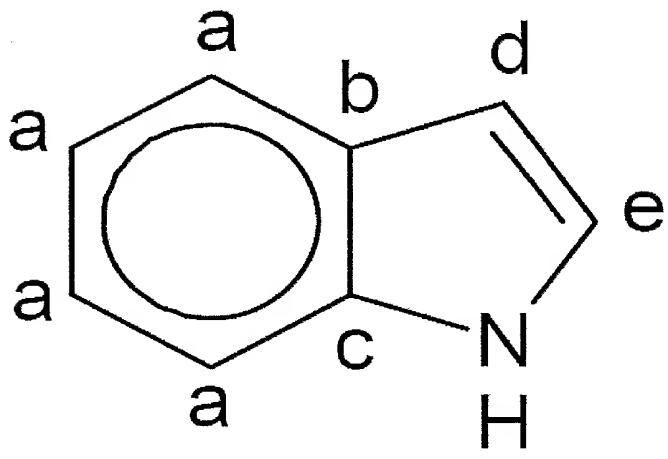
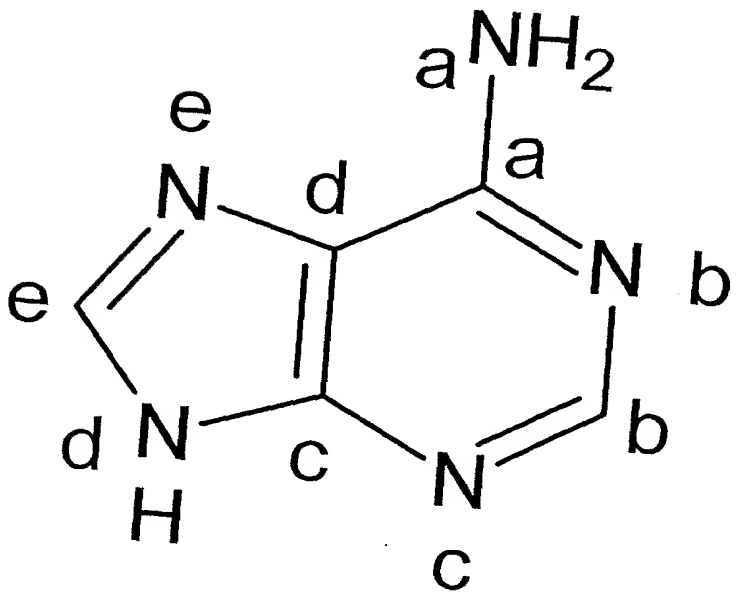


Fig. 75



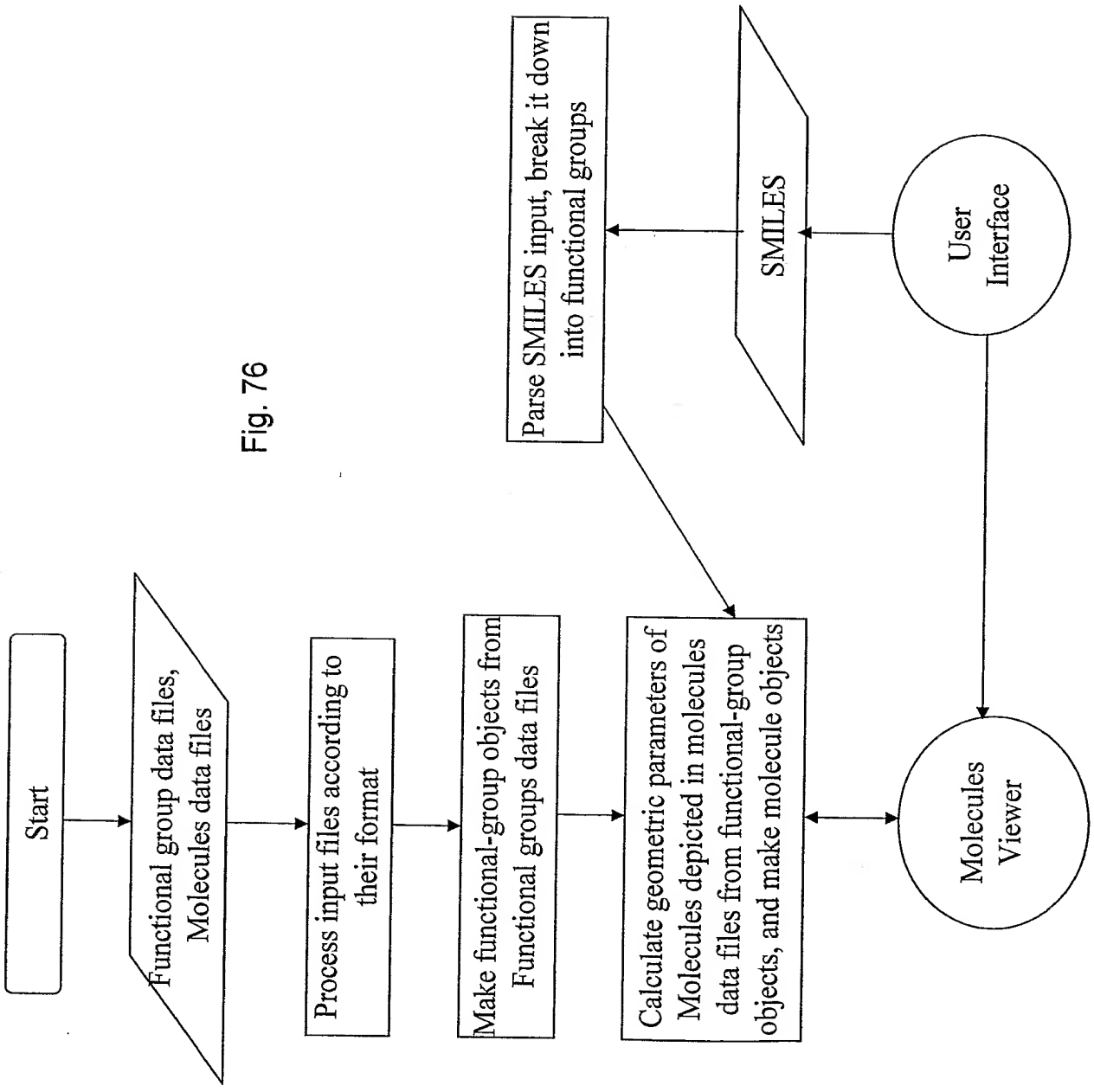
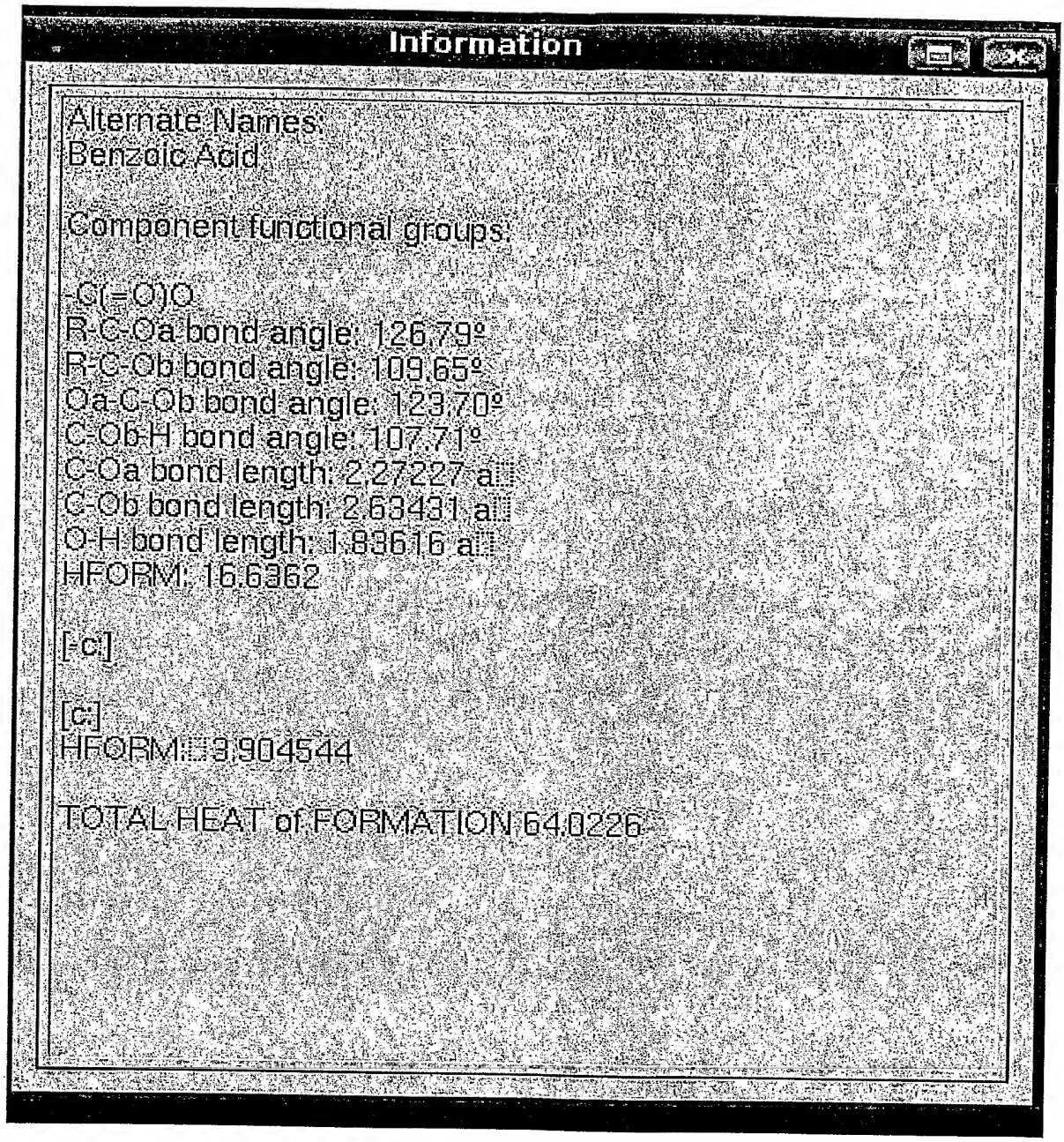

Start
Functional group data files, Molecules data files
Process input files according to their format
Make functional-group objects from Functional groups data files
Calculate geometric parameters of Molecules depicted in molecules data files from functional-group objects, and make molecule objects
Parse SMILES input, break it down into functional groups
SMILES
User Interface
Molecules Viewer

Fig. 76

Fig. 77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Alternate Names:
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Component functional groups:
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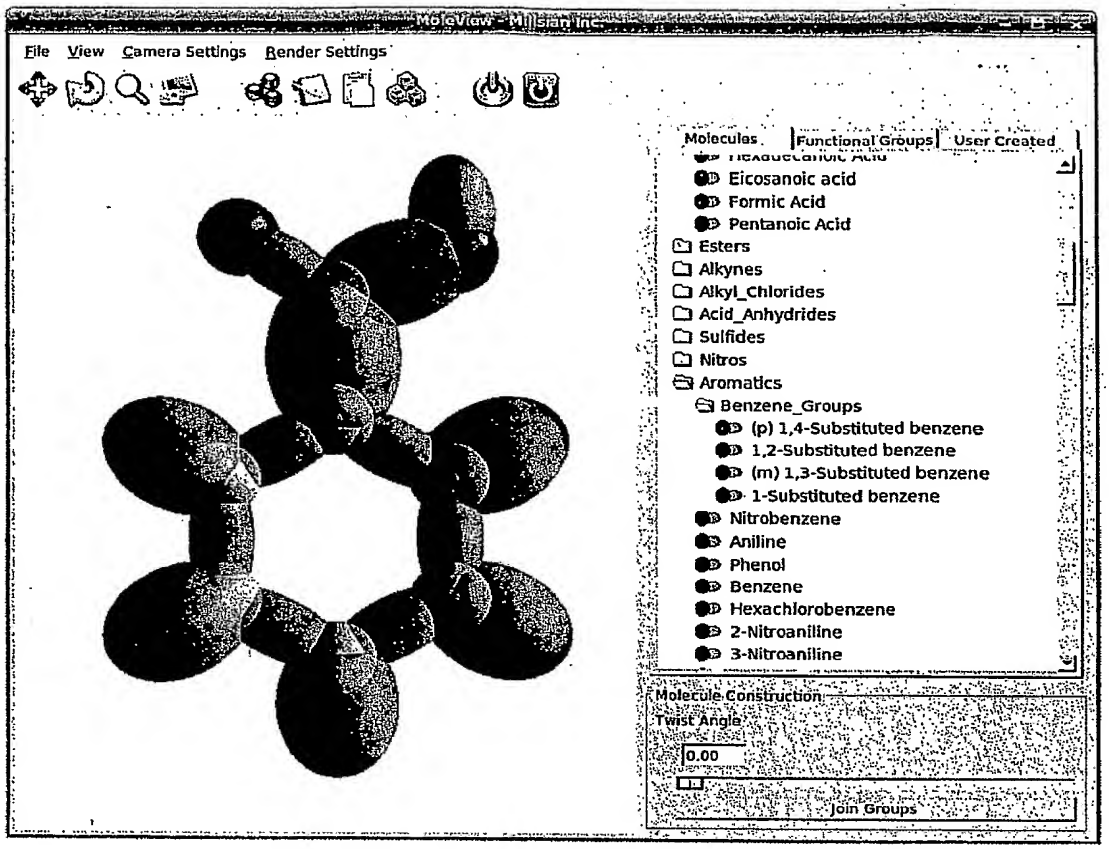
R-C-Ob bond angle: 109.65º
Oa-C-Ob bond angle: 123.70º
C-Ob-H bond angle: 107.71º
C-Oa bond length: 2.27227 a
C-Ob bond length: 2.63431 a
O-H bond length: 1.83616 a
HFORM: 16.6362
[-c]
[c]
HFORM: 3.904544
TOTAL HEAT of FORMATION 64.0226

Fig.78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User Created
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Pentanoic Acid
Esters
Alkynes
Alkyl_Chlorides
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Sulfides
Nitros
Aromatics
Benzene_Groups
(p) 1,4-Substituted benzene
1,2-Substituted benzene
(m) 1,3-Substituted benzene
1-Substituted benzene
Nitrobenzene
Aniline
Phenol
Benzene
Hexachlorobenzene
2-Nitroaniline
3-Nitroaniline
Molecule Construction
Twist Angle
0.00
Join Groups